

ARMY RESEARCH LABORATORY

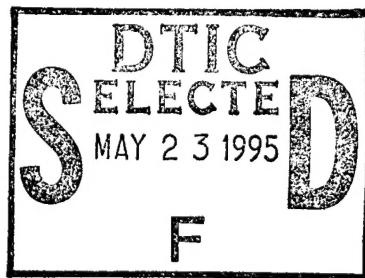


Predictions of the Spectra of the Rare-Earth Ions Ce^{3+} through Yb^{3+} in the Two Sites of $\text{Ca}_5(\text{PO}_4)_3\text{F}$

by Clyde A. Morrison

ARL-TR-708

April 1995



19950522 022

DTIC QUALITY INSPECTED 1

Approved for public release; distribution unlimited.

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorized documents.

Citation of manufacturer's or trade names does not constitute an official endorsement or approval of the use thereof.

Destroy this report when it is no longer needed. Do not return it to the originator.

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE April 1995		3. REPORT TYPE AND DATES COVERED Interim, from 1 June 1993 to 1 Nov 1994
4. TITLE AND SUBTITLE Predictions of the Spectra of the Rare-Earth Ions Ce^{3+} through Yb^{3+} in the Two Sites of $Ca_5(PO_4)_3F$			5. FUNDING NUMBERS PE: 611102.H44	
6. AUTHOR(S) Clyde A. Morrison				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory Attn: AMSRL-PS-AA 2800 Powder Mill Road Adelphi, MD 20783-1197			8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-708	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory 2800 Powder Mill Road Adelphi, MD 20783-1197			10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES AMS code: 21520406U6U01 ARL PR: 57E771				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) The results of fitting the experimental data on Er^{3+} in the two Ca^{2+} sites of $Ca_5(PO_4)_3F$ are used to predict the crystal-field parameters for the entire rare-earth series. These crystal-field parameters are then used along with the free-ion wavefunctions determined with aqueous parameters to determine a set of energy levels of the rare-earth ions Ce^{3+} through Yb^{3+} for both Ca^{2+} sites (Ca1 with C_3 symmetry and Ca2 with C_s symmetry) in $Ca_5(PO_4)_3F$. Also, the Judd-Ofelt parameters, Ω_k , are determined for each ion in the Ca1 and Ca2 sites, as well as the Zeeman g factors for the ground states.				
14. SUBJECT TERMS Spectra, rare earths, calcium fluoroapatite (fluorapatite)			15. NUMBER OF PAGES 74	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT UL	

Contents

1. Introduction	5
2. Smoothed Crystal-Field Parameters for Ce^{3+} Through Yb^{3+}	7
3. Judd-Ofelt Intensity Parameters	14
4. Predicted Energy Levels for Ca1 Site (C_3) and Ca2 Site (C_s)	15
5. Conclusion	53
References	54
Distribution	71

Appendices

A. Selection Rules for Dipole Electronic Transitions in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	55
B. Bibliography of Articles on Fluoroapatites	65

Tables

1. Data on $\text{Ca}_5(\text{PO}_4)_3\text{F}$	6
2. Monopole crystal-field components, A_{nm} ($\text{cm}^{-1}/\text{\AA}^n$), for Ca1 site, C_3 symmetry, in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	8
3. Monopole crystal-field components, A_{nm} ($\text{cm}^{-1}/\text{\AA}^n$), for Ca2 site, C_s symmetry	8
4. Experimental and best fit theoretical energy levels of Er^{3+} in C_3 site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	9
5. Experimental and best fit theoretical energy levels of Er^{3+} in C_s site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	11
6. Smoothed crystal-field parameters, B_{nm} (cm^{-1}), for C_3 site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	13
7. Smoothed crystal-field parameters B_{nm} (cm^{-1}) for C_s site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	13
8. Calculated Judd-Ofelt intensity parameters Ω_k (10^{-20} cm^2) of rare-earth ions in C_3 Ca site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	14
9. Calculated Judd-Ofelt intensity parameters Ω_k (10^{-20} cm^2) of rare-earth ions in C_s site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	14
10. Predicted g values of ground state of triply ionized rare-earth ions in two Ca sites in $\text{Ca}_5(\text{PO}_4)_3\text{F}$	15
11. Splitting (cm^{-1}) of 4I_J ($J = 15/2$ to $9/2$) for Er^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, LaF_3 , Y_2O_3	15
12. Predicted energy levels for Ce^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	16
13. Predicted energy levels for Pr^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	16
14. Predicted energy levels for Nd^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	17
15. Predicted energy levels for Pm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	19
16. Predicted energy levels for Sm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	20
17. Predicted energy levels for Eu^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	22
18. Predicted energy levels for Gd^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	23
19. Predicted energy levels for Tb^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	25
20. Predicted energy levels for Dy^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	27
21. Predicted energy levels for Ho^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	28
22. Predicted energy levels for Tm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	30
23. Predicted energy levels for Yb^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site	32

Tables (cont'd)

24.	Predicted energy levels for Ce^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	32
25.	Predicted energy levels for Pr^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	32
26.	Predicted energy levels for Nd^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	34
27.	Predicted energy levels for Pm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	36
28.	Predicted energy levels for Sm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	38
29.	Predicted energy levels for Eu^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	39
30.	Predicted energy levels for Gd^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	41
31.	Predicted energy levels for Tb^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	43
32.	Predicted energy levels for Dy^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	46
33.	Predicted energy levels for Ho^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	47
34.	Predicted energy levels for Tm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	50
35.	Predicted energy levels for Yb^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site	52

1. Introduction

Single crystals of $\text{Ca}_5(\text{PO}_4)_3\text{F}$ have been analyzed by x-ray diffraction, and the positions of all the ions in the unit cell have been determined [1,2]. The general space group information is given in table 1a. Since it is generally assumed that the rare-earth dopants replace the calcium ions, we see that of the 10 calcium ions in a unit cell, four are in the $4f$ position with C_3 symmetry and six are in the $6h$ position with C_s symmetry. The detailed x-ray data are given in table 1b. From the x-ray data in table 1b, the nearest neighbors to the Ca1, Ca2, and P sites were calculated; these are given in table 1c. These latter distances, particularly the Ca-Ca and Ca-P distances, are important in energy transfer considerations [3]. The crystal-field analysis assumes the crystal-field Hamiltonian of the form

$$H = \sum_{nm} B_{nm}^* \sum_i C_{nm}(\hat{r}_i), \quad (1)$$

where the B_{nm} are the crystal-field parameters, with $B_{nm}^* = (-1)^m B_{n-m}$ and $C_{nm} = \sqrt{4\pi / (2n+1)} Y_{nm}(\theta_i, \phi_i)$. The $Y_{nm}(\theta_i, \phi_i)$ are ordinary spherical harmonics with polar angles θ_i and ϕ_i . In equation (1), the sum on n covers the even integers 2, 4, and 6, and the sums on i cover the number of $4f$ electrons, N , in the triply ionized rare-earth ion configuration $4f^N$. The sum on m in equation (1) depends on which Ca ion site the rare-earth ion occupies. For the Ca1 site with C_3 symmetry, the crystal-field parameters are B_{20} , B_{40} , B_{43} , B_{60} , B_{63} , and B_{66} . If B_{43} is chosen as real, then B_{63} and B_{66} are in general complex, and eight crystal-field parameters result. For C_s symmetry, the number of crystal-field parameters is the same as for C_2 symmetry; that is, B_{n0} for $n = 2, 4, 6$ and B_{22} are real, and the remaining B_{nm} are complex, making a total of 14 crystal-field parameters (Morrison and Leavitt [4], pp 86, 87). Having to deal with such a large number of crystal-field parameters, plus the complexities of two different sites, means that we must have very good starting values for B_{nm} in the analysis of the optical data. In both C_3 symmetry and C_s symmetry, I have adopted the convention that the lowest even- n B_{nm} , with m not zero, is real and positive; that is, for C_3 , B_{43} is real and positive, and for C_s , B_{22} is real and positive (Morrison and Leavitt [4], pp 86, 87).

Accession For	
NTIS	CRA&I <input checked="" type="checkbox"/>
DTIC	TAB <input type="checkbox"/>
Unannounced <input type="checkbox"/>	
Justification	
By	
Distribution /	
Availability Codes	
Dist	Avail and/or Special
A-1	

Table 1. Data on $\text{Ca}_5(\text{PO}_4)_3\text{F}$.a. Crystallographic data: hexagonal C_{6h}^2 ($P6_3/m$), 176, $Z = 2$.

Ion	Site	Symmetry	x	y	z	q
O1	6h	C_s	x	y	1/4	-1.8
O2	6h	C_s	x	y	1/4	-1.8
O3	12i	C_1	x	y	z	-1.8
P	6h	C_s	x	y	1/4	4.2
Ca1	4f	C_3	1/3	2/3	z	2
Ca2	6h	C_s	x	y	1/4	2
F	2a	C_{3i}	0	0	1/4	-1

b. X-ray data.

a (Å)	c (Å)	O1		O2		O3		
		x	y	x	y	x	y	z
9.3973	6.8782	0.4849	0.3273	0.4667	0.5875	0.2575	0.3421	0.0705
9.3684	6.8841	0.329	0.484	0.589	0.466	0.348	0.259	0.0730

P		Ca1	Ca2		Reference
x	y	z	x	y	
0.36895	0.3985	0.0010	-0.00712	0.24227	Hughes et al (1989) [2]
0.400	0.369	0.001	0.246	-0.007	Wyckoff (1968) [1]

c. Distance (Å) to any number of nearest neighbors, N , to Ca1 (C_3), Ca2 (C_s), and P (C_s) sites in $\text{Ca}_5(\text{PO}_4)_3\text{F}$.

Ca1 site				Ca2 site				P site			
Ion	N	R (Å) ^a	R (Å) ^b	Ion	N	R (Å) ^a	R (Å) ^b	Ion	N	R (Å) ^a	R (Å) ^b
O1	3	2.399	2.408	F	1	2.311	2.338	O3	2	1.532	1.511
O2	3	2.457	2.442	O3	2	2.348	2.376	O1	1	1.537	1.523
O3	3	2.807	2.753	O2	1	2.374	2.340	O2	1	1.538	1.534
P	3	3.207	3.190	O3	2	2.501	2.495	Ca2	1	3.075	3.067
Ca1	2 ^c	3.44	3.45	O1	1	2.700	2.694	Ca1	2	3.207	3.190
Ca2	3	3.961	3.931	P	1	3.075	3.067				
				Ca1	2	3.961	3.931				
				Ca2	2	4.003	4.050				

^aHughes et al (1989) [2].^bWyckoff (1968) [1].^cAverage distance of two Ca1 ions.

2. Smoothed Crystal-Field Parameters for Ce^{3+} Through Yb^{3+}

The crystal-field parameters used in the first analysis are

$$B_{nm} = \rho_n A_{nm} , \quad (2)$$

where the radial factors ρ_n have been tabulated by Morrison and Leavitt [5], and the crystal-field components A_{nm} are calculated from the x-ray data [6]. For this analysis, I calculate only the monopole A_{nm} given by

$$A_{nm} = -e^2 \sum_j q_j \frac{C_{nm}(\hat{R}_j)}{R_j^{n+1}} , \quad (3)$$

where q_j is the effective charge (in units of electronic charge) on the ion at \mathbf{R}_j . The x-ray data given in table 1b, along with the effective charges in table 1a, are used to compute the A_{nm} for the C_3 site (table 2) and for the C_s site (table 3). The A_{nm} in table 2 have been rotated about the z-axis (crystal-line c-axis) so as to make A_{43} real and positive [4]. Similarly, the A_{nm} of table 3 have been rotated about the same axis so as to make A_{22} real and positive. The effective charges on the oxygen (-1.8) were chosen from the best fit to the experimental A_{nm} for triply ionized rare-earth ions in $\text{Y}_3\text{Sc}_2\text{Al}_3\text{O}_{12}$ [7]. The values of A_{nm} given in tables 2 and 3 with ρ_n for Er^{3+} were used in equation (1) to provide starting values for the C_3 and C_s spectra. The free-ion parameters were the same as used previously, and details of the fitting procedure are given elsewhere [8]. The irreducible representations for both C_s and C_3 symmetry are chosen from Koster et al [9]. The best fits to the experimental data for the C_3 site and the C_s site are given in tables 4 and 5. (These results have been previously reported but are included here for completeness [10].) Assuming that the A_{nm} are only host dependent, the best-fit B_{nm} can be used in equation (2) to produce experimental crystal-field components, A_{nm}^{exp} , by

$$A_{nm}^{\text{exp}} = B_{nm}(\text{Er})/\rho_n(\text{Er}) , \quad (4)$$

and by using equation (2) again, we have

$$B_{nm}(X) = B_{nm}(\text{Er}) \left[\rho_n(X)/\rho_n(\text{Er}) \right] , \quad (5)$$

where X is any rare-earth ion. This calculation has been done, and the results are given in table 6 for the Ca1 site (C_3 symmetry) and in table 7 for the Ca2 site (C_s symmetry) and are referred to as the smoothed crystal-field parameters.

Table 2. Monopole (point charge) crystal-field components, A_{nm} ($\text{cm}^{-1}/\text{\AA}^n$), for Ca1 site, C_3 symmetry, in $\text{Ca}_5(\text{PO}_4)_3\text{F}$.^a

$n m$	$\text{Re}A_{nm}^b$	$\text{Im}A_{nm}^b$	$\text{Re}A_{nm}^c$	$\text{Im}A_{nm}^c$
1 0	9184	—	11980	—
2 0	7142	—	7310	—
3 0	190	—	82.2	—
3 3	2330	2444	2129	-2802
4 0	-3795	—	-3900	—
4 3	1617	0	1761	0
5 0	-566	—	-596	—
5 3	-593	2714	-622	-2637
6 0	-755	—	-740	—
6 3	575	84.7	560	-164
6 6	-107	-246	-73.9	224
7 0	81.0	—	63.3	—
7 3	-55.6	1.50	-46.4	-147
7 6	-63.6	215	-83.4	-202

^aRotated so that A_{43} is real and positive.

^bWyckoff (1968) [1].

^cHughes et al (1989) [2].

Table 3. Monopole (point charge) crystal-field components, A_{nm} ($\text{cm}^{-1}/\text{\AA}^n$), for Ca2 site, C_s symmetry.^a

$n m$	$\text{Re}A_{nm}^b$	$\text{Im}A_{nm}^b$	$\text{Re}A_{nm}^c$	$\text{Im}A_{nm}^c$
1 1	-5252	-1142	-2852	-3017
2 0	7900	—	9481	—
2 2	1442	0	2110	0
3 1	270.7	3119	2822	-1716
3 3	-1980	-3204	1746	-3041
4 0	1850	—	2031	—
4 2	-2920	-1644	-2314	2428
4 4	829	2104	-487	-2189
5 1	-50.90	1924	1703	-1066
5 3	1150	441.6	-1123	462.7
5 5	-855.2	139.7	-574.0	639.5
6 0	47.3	—	90.8	—
6 2	293	-257	389	197
6 4	170	-103	171	-10.4
6 6	-169	-136	57.1	161
7 1	-3.344	99.30	103	-81.96
7 3	-139.8	-212.8	117.7	-216.8
7 5	-28.10	46.53	-50.28	10.45
7 7	-202.1	82.33	-19.47	-207.6

^aRotated so that A_{22} is real and positive.

^bWyckoff (1968) [1].

^cHughes et al (1989) [2].

Table 4. Experimental and best fit theoretical energy levels of Er^{3+} in C_3 site in $\text{Ca}_5(\text{PO}_4)_3\text{F}^a$

$2S+1L_J$ centroids (cm^{-1}) ^b	Level	Γ_n	Energy (cm^{-1})		Free-ion mixture (%)
			Theor.	Expt	
$4I_{15/2}$ (223)	1	$\Gamma_{4,5}$	-0.7	0.1	$99.91\ 4I_{15/2} + 0.04\ 4I_{13/2} + 0.01\ 4F_{9/2}$
	2	$2\Gamma_6$	19.2	18	$99.90\ 4I_{15/2} + 0.06\ 4I_{13/2} + 0.01\ 2H_{11/2}$
	3	$\Gamma_{4,5}$	43.1	41	$99.91\ 4I_{15/2} + 0.02\ 2H_{11/2} + 0.02\ 4I_{13/2}$
	4	$2\Gamma_6$	89.1	92	$99.89\ 4I_{15/2} + 0.06\ 4I_{13/2} + 0.02\ 2H_{11/2}$
	5	$\Gamma_{4,5}$	168.3	162	$99.87\ 4I_{15/2} + 0.07\ 4I_{13/2} + 0.02\ 2H_{11/2}$
	6	$2\Gamma_6$	373.9	376	$99.95\ 4I_{15/2} + 0.02\ 4I_{13/2} + 0.01\ 4F_{9/2}$
	7	$\Gamma_{4,5}$	445.0	—	$99.94\ 4I_{15/2} + 0.04\ 4I_{13/2} + 0.01\ 4I_{11/2}$
	8	$\Gamma_{4,5}$	560.7	—	$99.92\ 4I_{15/2} + 0.06\ 4I_{13/2} + 0.01\ 4F_{9/2}$
$4I_{13/2}$ (6688)	9	$\Gamma_{4,5}$	6532.0	6530	$99.86\ 4I_{13/2} + 0.04\ 4G_{9/2} + 0.03\ 4I_{9/2}$
	10	$2\Gamma_6$	6546.8	—	$99.80\ 4I_{13/2} + 0.07\ 4I_{11/2} + 0.03\ 4I_{15/2}$
	11	$\Gamma_{4,5}$	6571.3	6564	$99.71\ 4I_{13/2} + 0.17\ 4I_{11/2} + 0.04\ 4I_{9/2}$
	12	$\Gamma_{4,5}$	6619.0	6627	$99.51\ 4I_{13/2} + 0.41\ 4I_{11/2} + 0.02\ 4I_{9/2}$
	13	$\Gamma_{4,5}$	6779.6	6773	$99.80\ 4I_{13/2} + 0.12\ 4I_{15/2} + 0.03\ 4I_{11/2}$
	14	$2\Gamma_6$	6802.0	6806	$99.64\ 4I_{13/2} + 0.19\ 4I_{11/2} + 0.11\ 4I_{15/2}$
	15	$\Gamma_{4,5}$	6885.3	—	$99.76\ 4I_{13/2} + 0.17\ 4I_{11/2} + 0.05\ 4I_{15/2}$
$4I_{11/2}$ (10321)	16	$\Gamma_{4,5}$	10211.3	10211	$99.78\ 4I_{11/2} + 0.05\ 2G_{7/2} + 0.04\ 4I_{13/2}$
	17	$2\Gamma_6$	10230.1	10230	$99.68\ 4I_{11/2} + 0.11\ 4F_{9/2} + 0.08\ 4I_{9/2}$
	18	$\Gamma_{4,5}$	10268.6	10270	$99.74\ 4I_{11/2} + 0.08\ 4F_{9/2} + 0.08\ 4I_{9/2}$
	19	$\Gamma_{4,5}$	10352.8	10349	$99.29\ 4I_{11/2} + 0.38\ 4I_{13/2} + 0.24\ 4F_{9/2}$
	20	$\Gamma_{4,5}$	10399.5	—	$99.57\ 4I_{11/2} + 0.34\ 4I_{13/2} + 0.03\ 4I_{9/2}$
	21	$2\Gamma_6$	10422.6	10424	$99.42\ 4I_{11/2} + 0.31\ 4I_{9/2} + 0.20\ 4I_{13/2}$
$4I_{9/2}$ (12600)	22	$2\Gamma_6$	12403.0	12399	$99.60\ 4I_{9/2} + 0.17\ 4I_{11/2} + 0.14\ 4F_{9/2}$
	23	$\Gamma_{4,5}$	12500.0	12508	$99.59\ 4I_{9/2} + 0.08\ 4I_{11/2} + 0.07\ 4S_{3/2}$
	24	$\Gamma_{4,5}$	12622.4	12626	$99.70\ 4I_{9/2} + 0.09\ 4F_{9/2} + 0.06\ 4I_{11/2}$
	25	$2\Gamma_6$	12646.9	12645	$99.42\ 4I_{9/2} + 0.23\ 4F_{9/2} + 0.21\ 4I_{11/2}$
	26	$\Gamma_{4,5}$	12779.8	—	$99.63\ 4I_{9/2} + 0.13\ 4F_{9/2} + 0.10\ 2H_{11/2}$
$4F_{9/2}$ (15335)	27	$2\Gamma_6$	15142.4	15149	$99.45\ 4F_{9/2} + 0.26\ 4I_{9/2} + 0.13\ 2H_{11/2}$
	28	$\Gamma_{4,5}$	15296.8	15298	$99.46\ 4F_{9/2} + 0.16\ 2H_{11/2} + 0.15\ 4I_{9/2}$
	29	$\Gamma_{4,5}$	15369.1	—	$99.41\ 4F_{9/2} + 0.17\ 4I_{11/2} + 0.13\ 2H_{11/2}$
	30	$2\Gamma_6$	15406.2	15402	$99.58\ 4F_{9/2} + 0.14\ 2H_{11/2} + 0.09\ 4I_{9/2}$
	31	$\Gamma_{4,5}$	15446.0	15440	$99.48\ 4F_{9/2} + 0.22\ 2H_{11/2} + 0.13\ 4I_{11/2}$
$4S_{3/2}$ (18411)	32	$2\Gamma_6$	18305.2	18307	$96.46\ 4S_{3/2} + 3.37\ 2H_{11/2} + 0.03\ 4I_{9/2}$
	33	$\Gamma_{4,5}$	18445.8	18442	$94.03\ 4S_{3/2} + 5.70\ 2H_{11/2} + 0.08\ 4I_{9/2}$
$2H_{11/2}$ (19094)	34	$\Gamma_{4,5}$	19009.8	19013	$97.44\ 2H_{11/2} + 1.24\ 4S_{3/2} + 0.74\ 4F_{7/2}$
	35	$\Gamma_{4,5}$	19041.7	19048	$97.66\ 2H_{11/2} + 1.26\ 4S_{3/2} + 0.64\ 4F_{7/2}$
	36	$2\Gamma_6$	19085.4	19082	$97.45\ 2H_{11/2} + 1.35\ 4S_{3/2} + 0.83\ 4F_{7/2}$
	37	$2\Gamma_6$	19115.2	19106	$96.85\ 2H_{11/2} + 1.98\ 4S_{3/2} + 0.86\ 4F_{7/2}$
	38	$\Gamma_{4,5}$	19148.8	19144	$99.25\ 2H_{11/2} + 0.38\ 4S_{3/2} + 0.25\ 4F_{7/2}$
	39	$\Gamma_{4,5}$	19186.3	19207	$96.06\ 2H_{11/2} + 2.85\ 4S_{3/2} + 0.80\ 4F_{7/2}$
$4F_{7/2}$ (20458)	40	$\Gamma_{4,5}$	20290.8	20285	$98.85\ 4F_{7/2} + 0.55\ 2H_{11/2} + 0.17\ 4F_{5/2}$
	41	$\Gamma_{4,5}$	20422.1	20422	$97.33\ 4F_{7/2} + 1.39\ 2H_{11/2} + 1.04\ 4F_{5/2}$
	42	$2\Gamma_6$	20489.2	20492	$97.79\ 4F_{7/2} + 1.66\ 2H_{11/2} + 0.24\ 4F_{3/2}$
	43	$\Gamma_{4,5}$	20629.6	20630	$98.93\ 4F_{7/2} + 0.46\ 2H_{11/2} + 0.34\ 4F_{5/2}$
$4F_{5/2}$ (22191)	44	$2\Gamma_6$	22118.3	22117	$87.34\ 4F_{5/2} + 12.28\ 4F_{3/2} + 0.09\ 2G_{7/2}$
	45	$\Gamma_{4,5}$	22163.1	22164	$97.89\ 4F_{5/2} + 1.27\ 4F_{7/2} + 0.28\ 2H_{11/2}$
	46	$\Gamma_{4,5}$	22249.5	22251	$99.23\ 4F_{5/2} + 0.20\ 4F_{7/2} + 0.16\ 4G_{9/2}$

Table 4 (cont'd). Experimental and best fit theoretical energy levels of Er^{3+} in C_3 site in $\text{Ca}_5(\text{PO}_4)_3\text{F}^a$

$2S+1L_J$ centroids (cm^{-1}) ^b	Level	Γ_n	Energy (cm^{-1})		Free-ion mixture (%)
			Theor.	Expt	
$^4F_{3/2}$ (22639)	47	$^2\Gamma_6$	22593.9	—	$87.09\ ^4F_{3/2} + 12.25\ ^4F_{5/2} + 0.25\ ^4G_{9/2}$
	48	$\Gamma_{4,5}$	22741.7	22742	$99.35\ ^4F_{3/2} + 0.26\ ^4F_{5/2} + 0.13\ ^2G_{7/2}$
$^2G_{9/2}$ (24651)	49	$^2\Gamma_6$	24451.7	24448	$99.33\ ^2G_{9/2} + 0.45\ ^2K_{15/2} + 0.07\ ^4G_{11/2}$
	50	$\Gamma_{4,5}$	24568.0	24575	$97.92\ ^2G_{9/2} + 1.53\ ^4G_{11/2} + 0.38\ ^2K_{15/2}$
	51	$^2\Gamma_6$	24678.3	24678	$98.83\ ^2G_{9/2} + 0.71\ ^4G_{11/2} + 0.22\ ^2K_{15/2}$
	52	$\Gamma_{4,5}$	24693.9	24695	$98.73\ ^2G_{9/2} + 0.84\ ^4G_{11/2} + 0.20\ ^2K_{15/2}$
	53	$\Gamma_{4,5}$	24764.6	—	$97.80\ ^2G_{9/2} + 1.46\ ^4G_{11/2} + 0.50\ ^2K_{15/2}$
$^4G_{11/2}$ (26367)	54	$\Gamma_{4,5}$	26261.1	26261	$96.99\ ^4G_{11/2} + 1.86\ ^2G_{9/2} + 0.55\ ^2K_{15/2}$
	55	$^2\Gamma_6$	26272.9	26278	$98.56\ ^4G_{11/2} + 0.90\ ^4G_{9/2} + 0.37\ ^2K_{15/2}$
	56	$\Gamma_{4,5}$	26321.2	26321	$97.03\ ^4G_{11/2} + 1.24\ ^2G_{9/2} + 1.02\ ^2K_{15/2}$
	57	$^2\Gamma_6$	26407.6	26408	$94.90\ ^4G_{11/2} + 1.95\ ^4G_{9/2} + 1.93\ ^2K_{15/2}$
	58	$\Gamma_{4,5}$	26435.9	26425	$97.84\ ^4G_{11/2} + 1.24\ ^2K_{15/2} + 0.39\ ^4G_{9/2}$
$^4G_{9/2}$ 27479 ^b	59	$\Gamma_{4,5}$	26478.5	—	$94.47\ ^4G_{11/2} + 4.11\ ^2K_{15/2} + 0.47\ ^4G_{9/2}$
	60	$\Gamma_{4,5}$	27352.4	—	$89.44\ ^2K_{15/2} + 5.93\ ^4G_{11/2} + 3.43\ ^4G_{9/2}$
$^2K_{15/2}$ 27800 ^b	61	$^2\Gamma_6$	27421.7	—	$90.71\ ^2K_{15/2} + 4.32\ ^4G_{9/2} + 2.71\ ^4G_{11/2}$
	62	$\Gamma_{4,5}$	27438.4	—	$90.30\ ^4G_{9/2} + 4.66\ ^2K_{15/2} + 4.56\ ^2G_{7/2}$
$^2G_{7/2}$ 27981 ^a	63	$\Gamma_{4,5}$	27480.8	—	$97.12\ ^4G_{9/2} + 1.86\ ^2G_{7/2} + 0.50\ ^4G_{11/2}$
	64	$^2\Gamma_6$	27493.0	—	$86.66\ ^4G_{9/2} + 7.05\ ^2G_{7/2} + 4.07\ ^2K_{15/2}$
	65	$\Gamma_{4,5}$	27505.4	—	$95.41\ ^4G_{9/2} + 2.35\ ^2G_{7/2} + 1.12\ ^2K_{15/2}$
	66	$^2\Gamma_6$	27530.3	—	$95.29\ ^4G_{9/2} + 3.03\ ^2K_{15/2} + 0.80\ ^4G_{11/2}$
	67	$\Gamma_{4,5}$	27587.2	—	$96.28\ ^2K_{15/2} + 1.96\ ^2G_{7/2} + 0.79\ ^4G_{9/2}$
	68	$\Gamma_{4,5}$	27807.5	—	$94.16\ ^2K_{15/2} + 2.67\ ^4G_{9/2} + 2.31\ ^2G_{7/2}$
	69	$\Gamma_{4,5}$	27954.2	—	$90.72\ ^2G_{7/2} + 7.35\ ^2K_{15/2} + 1.72\ ^4G_{9/2}$
	70	$^2\Gamma_6$	27982.5	—	$86.97\ ^2K_{15/2} + 10.40\ ^2G_{7/2} + 2.37\ ^4G_{9/2}$
	71	$\Gamma_{4,5}$	28020.8	—	$84.69\ ^2G_{7/2} + 13.35\ ^2K_{15/2} + 1.40\ ^4G_{9/2}$
	72	$\Gamma_{4,5}$	28052.0	—	$90.48\ ^2G_{7/2} + 5.06\ ^2K_{15/2} + 4.06\ ^4G_{9/2}$
	73	$^2\Gamma_6$	28078.5	—	$62.33\ ^2K_{15/2} + 33.96\ ^2G_{7/2} + 3.52\ ^4G_{9/2}$
	74	$^2\Gamma_6$	28105.9	—	$49.83\ ^2K_{15/2} + 45.42\ ^2G_{7/2} + 4.35\ ^4G_{9/2}$
	75	$\Gamma_{4,5}$	28152.2	—	$87.77\ ^2K_{15/2} + 11.67\ ^2G_{7/2} + 0.28\ ^4G_{11/2}$
	76	$\Gamma_{4,5}$	28175.4	—	$92.35\ ^2K_{15/2} + 6.99\ ^2G_{7/2} + 0.43\ ^4G_{9/2}$

With an rms = $4.832\ \text{cm}^{-1}$ B_{nm} (cm^{-1}) are $B_{20} = 1281$, $B_{40} = -1600$, $B_{43} = 563$, $B_{60} = -727$, $B_{63} = 505 + i273$, $B_{66} = 87.8 - i279$, and $\text{Im}B_{66} = -277$.

^aGruber et al (1994) [10]. The Γ_n labels are from Koster et al (1963) [9].

^bAqueous centroids.

Table 5. Experimental and best fit theoretical energy levels of Er^{3+} in C_s site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$.^a

$2S+1L_J$ centroids (cm^{-1}) ^b	Level	Energy (cm^{-1})		Free-ion mixture (%)
		Theor.	Expt	
$4I_{15/2}$ (328)	1	5.9	0	$99.90\ 4I_{15/2} + 0.03\ 4I_{13/2} + 0.03\ 2H_{11/2}$
	2	141.5	139	$99.90\ 4I_{15/2} + 0.05\ 4I_{13/2} + 0.02\ 2H_{11/2}$
	3	186.9	194	$99.92\ 4I_{15/2} + 0.03\ 4I_{13/2} + 0.02\ 2H_{11/2}$
	4	257.6	256	$99.92\ 4I_{15/2} + 0.02\ 4I_{13/2} + 0.02\ 4F_{9/2}$
	5	319.6	314	$99.92\ 4I_{15/2} + 0.04\ 4I_{13/2} + 0.01\ 4F_{9/2}$
	6	441.5	—	$99.93\ 4I_{15/2} + 0.02\ 4I_{13/2} + 0.01\ 4F_{9/2}$
	7	522.3	—	$99.91\ 4I_{15/2} + 0.04\ 4I_{13/2} + 0.03\ 4F_{9/2}$
	8	653.7	662	$99.95\ 4I_{15/2} + 0.03\ 4I_{13/2} + 0.01\ 2H_{11/2}$
$4I_{13/2}$ (6804)	9	6578.8	6583	$99.76\ 4I_{13/2} + 0.13\ 4I_{11/2} + 0.03\ 4G_{9/2}$
	10	6678.0	6667	$99.67\ 4I_{13/2} + 0.22\ 4I_{11/2} + 0.03\ 4G_{9/2}$
	11	6710.5	6713	$99.84\ 4I_{13/2} + 0.07\ 4I_{11/2} + 0.03\ 4I_{15/2}$
	12	6760.5	6773	$99.67\ 4I_{13/2} + 0.21\ 4I_{11/2} + 0.05\ 4I_{15/2}$
	13	6856.6	—	$99.85\ 4I_{13/2} + 0.04\ 4I_{15/2} + 0.03\ 4I_{11/2}$
	14	6906.6	6906	$99.71\ 4I_{13/2} + 0.17\ 4I_{11/2} + 0.06\ 4I_{15/2}$
	15	7045.2	7038	$99.80\ 4I_{13/2} + 0.10\ 4I_{11/2} + 0.03\ 4I_{15/2}$
$4I_{11/2}$ (10351)	16	10216.4	—	$99.59\ 4I_{11/2} + 0.15\ 4I_{13/2} + 0.12\ 4I_{9/2}$
	17	10279.3	10291	$99.61\ 4I_{11/2} + 0.18\ 4I_{9/2} + 0.07\ 4I_{13/2}$
	18	10308.9	10312	$99.70\ 4I_{11/2} + 0.11\ 4I_{13/2} + 0.06\ 4F_{9/2}$
	19	10359.4	10349	$99.69\ 4I_{11/2} + 0.15\ 4I_{13/2} + 0.07\ 4F_{9/2}$
	20	10399.0	—	$99.54\ 4I_{11/2} + 0.28\ 4I_{13/2} + 0.06\ 4I_{9/2}$
	21	10495.5	10491	$99.57\ 4I_{11/2} + 0.17\ 4I_{13/2} + 0.14\ 4I_{9/2}$
$4I_{9/2}$ (12605)	22	12431.7	—	$99.66\ 4I_{9/2} + 0.17\ 4F_{9/2} + 0.04\ 4I_{11/2}$
	23	12544.0	12552	$99.63\ 4I_{9/2} + 0.12\ 4I_{11/2} + 0.09\ 4F_{9/2}$
	24	12579.3	12580	$99.50\ 4I_{9/2} + 0.21\ 4I_{11/2} + 0.10\ 4F_{9/2}$
	25	12654.7	12646	$99.49\ 4I_{9/2} + 0.13\ 4I_{11/2} + 0.12\ 4F_{9/2}$
	26	12754.7	—	$99.49\ 4I_{9/2} + 0.25\ 4F_{9/2} + 0.10\ 4I_{11/2}$
$4F_{9/2}$ (15420)	27	15237.0	15244	$99.18\ 4F_{9/2} + 0.37\ 4I_{9/2} + 0.21\ 2H_{11/2}$
	28	15302.7	15298	$99.45\ 4F_{9/2} + 0.24\ 2H_{11/2} + 0.07\ 4I_{11/2}$
	29	15434.3	15437	$99.34\ 4F_{9/2} + 0.30\ 2H_{11/2} + 0.13\ 4I_{9/2}$
	30	15512.1	15509	$99.45\ 4F_{9/2} + 0.19\ 2H_{11/2} + 0.14\ 4I_{9/2}$
	31	15576.7	15575	$99.71\ 4F_{9/2} + 0.06\ 4I_{9/2} + 0.05\ 2H_{11/2}$
$4S_{3/2}$ (18432)	32	18300.4	18293	$95.09\ 4S_{3/2} + 4.61\ 2H_{11/2} + 0.05\ 4I_{9/2}$
	33	18448.8	18457	$92.09\ 4S_{3/2} + 7.54\ 2H_{11/2} + 0.08\ 4F_{7/2}$
$2H_{11/2}$ (19181)	34	19078.3	19087	$97.81\ 2H_{11/2} + 1.21\ 4S_{3/2} + 0.72\ 4F_{7/2}$
	35	19137.2	19141	$97.76\ 2H_{11/2} + 1.75\ 4S_{3/2} + 0.21\ 4F_{7/2}$
	36	19184.2	19179	$97.92\ 2H_{11/2} + 1.20\ 4S_{3/2} + 0.29\ 4F_{7/2}$
	37	19217.0	19198	$93.11\ 2H_{11/2} + 5.54\ 4S_{3/2} + 0.89\ 4F_{7/2}$
	38	19263.1	19259	$97.86\ 2H_{11/2} + 1.15\ 4S_{3/2} + 0.54\ 4F_{7/2}$
	39	19280.4	19295	$97.10\ 2H_{11/2} + 1.42\ 4S_{3/2} + 1.03\ 4F_{7/2}$
$4F_{7/2}$ (20552)	40	20346.0	20347	$98.36\ 4F_{7/2} + 0.86\ 2H_{11/2} + 0.25\ 4F_{5/2}$
	41	20516.7	20534	$97.59\ 4F_{7/2} + 1.20\ 2H_{11/2} + 0.57\ 4F_{5/2}$
	42	20617.6	20601	$98.18\ 4F_{7/2} + 0.70\ 2H_{11/2} + 0.60\ 4F_{5/2}$
	43	20696.7	20695	$97.93\ 4F_{7/2} + 0.99\ 2H_{11/2} + 0.53\ 4F_{5/2}$
$4F_{5/2}$ (22204)	44	22125.6	22114	$93.50\ 4F_{5/2} + 5.47\ 4F_{3/2} + 0.44\ 4F_{7/2}$
	45	22162.7	22164	$85.15\ 4F_{5/2} + 13.08\ 4F_{3/2} + 1.02\ 4F_{7/2}$
	46	22245.6	22256	$95.44\ 4F_{5/2} + 3.48\ 4F_{3/2} + 0.63\ 4F_{7/2}$

Table 5 (cont'd). Experimental and best fit theoretical energy levels of Er^{3+} in C_5 site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$.^a

$^{2S+1}L_J$ centroids (cm^{-1}) ^b	Level	Energy (cm^{-1})		Free-ion mixture (%)
		Theor.	Expt	
$^4F_{3/2}$ (22599)	47	22551.6	22550	$82.27 ^4F_{3/2} + 16.92 ^4F_{5/2} + 0.37 ^4F_{7/2}$
	48	22740.5	22742	$94.18 ^4F_{3/2} + 5.22 ^4F_{5/2} + 0.16 ^4F_{7/2}$
$^2G_{9/2}$ (24556)	49	24394.2	24401	$98.49 ^2G_{9/2} + 0.70 ^4G_{11/2} + 0.55 ^2K_{15/2}$
	50	24459.9	24448	$98.23 ^2G_{9/2} + 0.93 ^4G_{11/2} + 0.54 ^2K_{15/2}$
	51	24543.5	—	$98.82 ^2G_{9/2} + 0.56 ^4G_{11/2} + 0.37 ^2K_{15/2}$
	52	24582.9	24588	$97.65 ^2G_{9/2} + 1.38 ^4G_{11/2} + 0.61 ^2K_{15/2}$
	53	24673.4	—	$98.20 ^2G_{9/2} + 0.84 ^4G_{11/2} + 0.70 ^2K_{15/2}$
$^4G_{11/2}$ (26398)	54	26214.2	26206	$97.91 ^4G_{11/2} + 1.22 ^4G_{9/2} + 0.54 ^2K_{15/2}$
	55	26261.1	26265	$98.60 ^4G_{11/2} + 0.56 ^4G_{9/2} + 0.38 ^2K_{15/2}$
	56	26369.2	26364	$95.65 ^4G_{11/2} + 1.59 ^2G_{9/2} + 1.33 ^2K_{15/2}$
	57	26465.4	26464	$96.38 ^4G_{11/2} + 1.74 ^4G_{9/2} + 0.97 ^2K_{15/2}$
	58	26520.5	26523	$95.12 ^4G_{11/2} + 1.86 ^4G_{9/2} + 1.67 ^2K_{15/2}$
	59	26560.4	26569	$96.66 ^4G_{11/2} + 1.35 ^2K_{15/2} + 0.82 ^2G_{9/2}$
$^4G_{9/2}$ 27479 ^b $^2K_{15/2}$ 27800 ^b $^2G_{7/2}$ 27981 ^b	60	27293.8	—	$91.95 ^2K_{15/2} + 3.59 ^4G_{9/2} + 1.75 ^4G_{11/2}$
	61	27433.1	—	$82.41 ^4G_{9/2} + 8.44 ^2K_{15/2} + 7.16 ^2G_{7/2}$
	62	27443.6	—	$84.89 ^4G_{9/2} + 7.75 ^2G_{7/2} + 6.53 ^2K_{15/2}$
	63	27474.4	—	$58.33 ^4G_{9/2} + 38.42 ^2K_{15/2} + 1.95 ^2G_{7/2}$
	64	27518.1	—	$77.33 ^4G_{9/2} + 14.88 ^2K_{15/2} + 6.33 ^2G_{7/2}$
	65	27527.1	—	$56.67 ^4G_{9/2} + 37.59 ^2K_{15/2} + 3.31 ^2G_{7/2}$
	66	27559.4	—	$92.19 ^4G_{9/2} + 4.31 ^2K_{15/2} + 1.63 ^4G_{11/2}$
	67	27609.3	—	$89.97 ^2K_{15/2} + 6.58 ^4G_{9/2} + 1.70 ^2G_{7/2}$
	68	27647.8	—	$93.68 ^2K_{15/2} + 2.83 ^4G_{9/2} + 2.11 ^2G_{7/2}$
	69	27830.8	—	$87.20 ^2K_{15/2} + 11.45 ^2G_{7/2} + 0.73 ^4G_{9/2}$
	70	27923.5	—	$90.24 ^2K_{15/2} + 8.26 ^2G_{7/2} + 1.01 ^4G_{9/2}$
	71	27998.8	—	$89.64 ^2G_{7/2} + 5.37 ^2K_{15/2} + 4.62 ^4G_{9/2}$
	72	28043.4	—	$74.37 ^2G_{7/2} + 16.79 ^2K_{15/2} + 8.24 ^4G_{9/2}$
	73	28084.0	—	$82.50 ^2G_{7/2} + 13.36 ^2K_{15/2} + 3.46 ^4G_{9/2}$
	74	28110.4	—	$81.16 ^2G_{7/2} + 10.37 ^2K_{15/2} + 7.81 ^4G_{9/2}$
	75	28209.0	—	$84.17 ^2K_{15/2} + 14.66 ^2G_{7/2} + 0.44 ^2G_{9/2}$
	76	28526.2	—	$97.54 ^2K_{15/2} + 2.10 ^2G_{7/2} + 0.26 ^4G_{11/2}$

The B_{nm} (cm^{-1}) are $B_{20} = 1406$, $B_{22} = 236$, $B_{40} = 744$, $B_{42} = -1306 - i587$, $\text{Im}B_{42} = 50.5 + i566$, $B_{60} = -42$, $B_{62} = 203 - i225$, $B_{64} = 397 + i165$, and $B_{66} = -131 + i123$. The rms = 7.892 cm^{-1} .

^aGruber et al (1994) [10]. All levels are the $\Gamma_3 + \Gamma_4$ Kramers doublets in the notation of Koster et al (1963) [9].

Table 6. Smoothed crystal-field parameters, B_{nm} (cm^{-1}), for C_3 site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$.

Ion	B_{20}	B_{40}	B_{43}	B_{60}	$\text{Re}B_{63}$	$\text{Im}B_{63}$	$\text{Re}B_{66}$	$\text{Im}B_{66}$
A_{nm}	7509	-3878	1365	-740	514	278	89.4	-284
Ce	1382	-2922	1028	-1801	1251	676	218	-691
Pr	1318	-2507	882	-1388	964	521	168	-533
Nd	1281	-2240	788	-1376	817	442	142	-451
Pm	1261	-2070	729	-1052	731	395	127	-404
Sm	1252	-1958	689	-977	679	367	118	-375
Eu	1251	-1875	660	-925	643	347	112	-355
Gd	1252	-1806	635	-878	610	330	106	-337
Tb	1256	-1741	613	-831	577	312	100	-319
Dy	1262	-1683	592	-785	545	295	94.8	-301
Ho	1270	-1635	575	-749	520	281	90.4	-287
Er	1281	-1600	563	-727	505	273	87.8	-279
Tm	1293	-1572	553	-714	496	268	86.2	-274
Yb	1304	-1527	537	-675	469	253	81.5	-259

Table 7. Smoothed crystal-field parameters B_{nm} (cm^{-1}) for C_s site in $\text{Ca}_5(\text{PO}_4)_3\text{F}$.

Ion	B_{20}	B_{22}	B_{40}	$\text{Re}B_{42}$	$\text{Im}B_{42}$	$\text{Re}B_{44}$	$\text{Im}B_{44}$
A_{nm}	8242	1383	1803	-3165	-1423	122	1372
Ce	1517	255	1359	-2385	-1072	92.2	1034
Pr	1447	243	1166	-2046	-920	79.1	887
Nd	1406	236	1342	-1828	-822	70.7	792
Pm	1384	232	963	-1690	-760	65.3	732
Sm	1375	231	910	-1598	-718	61.8	693
Eu	1373	230	872	-1531	-688	59.2	663
Gd	1375	231	840	-1474	-662	57.0	639
Tb	1379	231	810	-1421	-639	55.0	616
Dy	1385	233	783	-1374	-618	53.1	595
Ho	1394	234	760	-1335	-600	51.6	578
Er	1406	236	744	-1306	-587	50.5	566
Tm	1419	238	731	-1283	-577	49.6	556
Yb	1432	240	710	-1246	-560	48.2	540

Ion	B_{60}	$\text{Re}B_{62}$	$\text{Im}B_{62}$	$\text{Re}B_{64}$	$\text{Im}B_{64}$	$\text{Re}B_{66}$	$\text{Im}B_{66}$
A_{nm}	-42.7	207	-229	404	168	-133	125
Ce	-104	503	-557	983	409	-325	305
Pr	-80.2	387	-429	758	315	-250	235
Nd	-67.9	328	-364	642	267	-212	199
Pm	-60.8	294	-326	574	239	-190	178
Sm	-56.5	273	-302	534	222	-176	165
Eu	-53.4	258	-286	505	210	-167	157
Gd	-50.7	245	-272	480	199	-158	148
Tb	-48.0	232	-257	454	189	-150	141
Dy	-45.4	219	-243	429	178	-142	133
Ho	-43.3	209	-232	409	170	-135	127
Er	-42.0	203	-225	397	165	-131	123
Tm	-41.2	199	-221	390	162	-129	121
Yb	-39.0	188	-209	368	153	-122	114

3. Judd-Ofelt Intensity Parameters

The Judd-Ofelt parameters for the Ca1 (C₃) site and the Ca2 (C_s) site have been calculated and are given in tables 8 and 9, respectively. In the calculation of the Judd-Ofelt parameters, the formula

$$\Omega_t = 28(2t+1) \sum_k S_k^2 N_k^2(t), \quad t = 2, 4, \text{ and } 6, \quad (6)$$

from Leavitt and Morrison [11] has been used. The $N_k(t)$ are given there, and

$$S_k^2 = \frac{1}{2k+1} \left[A_{k0}^2 + 2 \sum_{m=1}^k |A_{km}|^2 \right], \quad k = 1, 3, 5, \text{ and } 7. \quad (7)$$

Table 8. Calculated Judd-Ofelt intensity parameters Ω_k (10^{-20} cm²) of rare-earth ions in C₃ Ca site in Ca₅(PO₄)₃F.^a

Ion	Ω_2	Ω_4	Ω_6
Ce	22.46	12.95	58.25
Pr	13.61	6.530	24.83
Nd	10.13	4.228	13.63
Pm	8.541	3.253	10.47
Sm	7.769	2.771	8.671
Eu	6.143	2.105	6.131
Gd	4.754	1.575	4.233
Tb	10.06	3.068	10.28
Dy	7.136	2.110	6.376
Ho	5.742	1.648	4.654
Er	5.623	1.567	4.390
Tm	5.583	1.517	4.241
Yb	4.671	1.229	3.231

^aHughes et al (1989) [2].

Table 9. Calculated Judd-Ofelt intensity parameters Ω_k (10^{-20} cm²) of rare-earth ions in C_s site in Ca₅(PO₄)₃F.^a

Ion	Ω_2	Ω_4	Ω_6
Ce	13.89	18.60	46.88
Pr	8.19	9.373	20.03
Nd	6.68	6.162	11.00
Pm	4.983	4.792	8.450
Sm	4.456	4.041	6.990
Eu	3.525	3.030	4.954
Gd	2.737	2.230	3.426
Tb	5.498	4.772	8.228
Dy	3.936	3.204	5.118
Ho	3.180	2.472	3.739
Er	3.096	2.364	3.525
Tm	3.058	2.304	3.0402
Yb	2.563	1.852	2.594

^aHughes et al (1989) [2].

4. Predicted Energy Levels for Ca1 Site (C_3) and Ca2 Site (C_s)

The smoothed crystal-field parameters for the Ca1 site given in table 6 have been used in the calculation of the energy levels of the entire triply ionized rare-earth series Ce^{3+} through Yb^{3+} ; these energy levels are given in tables 6 through 23. The smoothed crystal-field parameters for the Ca2 site given in table 7 have been used for a similar calculation, with the results given in tables 24 through 35. The g values for those ions having doublet ground states have been calculated and are given in table 10.

Table 10. Predicted g values of ground state of triply ionized rare-earth ions in two Ca sites in $Ca_5(PO_4)_3F$.

Ion	C_3		C_s^a		
	g_{\parallel}	g_{\perp}	g_{\parallel}	$g_{\perp 1}^b$	$g_{\perp 2}^b$
Ce	-3.6897	0.317	2.467	1.629	0.326
Pr ^c	—	—	—	—	—
Nd	4.556	0.930	2.210	3.660	0.934
Pm	1.544	0	—	—	—
Sm	1.079	0.255	-0.345	0.736	0.134
Eu ^c	—	—	—	—	—
Gd	1.994	7.979	0.931	12.845	1.857
Tb ^c	—	—	—	—	—
Dy	-14.422	0.276	-19.487	0.011	0.007
Ho	16.537	0	—	—	—
Er	0.694	8.737	-0.532	16.159	1.027
Tm ^c	—	—	—	—	—
Yb	6.645	—	-0.012	7.056	0.097

^aIn C_s symmetry, g values exist only for rare-earth elements with an odd number of f electrons.

^b $g_{\perp 1}$ and $g_{\perp 2}$ are magnitudes of principal g factors in a, b plane (g_{\parallel} is parallel to c -axis).

^cThese ions have singlet ground states in C_3 sites as well as C_s sites.

Table 11. Splitting (cm^{-1}) of 4I_J ($J = 15/2$ to $9/2$) for Er^{3+} in $Ca_5(PO_4)_3F$, LaF_3 , Y_2O_3 .

State	$Ca_5(PO_4)_3F$		LaF_3^b	$Y_2O_3^c$
	C_3^a	C_s^a		
$^4I_{15/2}$	562	662	443	510
$^4I_{13/2}$	353	455	219	357
$^4I_{11/2}$	212	280	94	186
$^4I_{9/2}$	377	323	311	280

^aThis work, table 5, for C_3 site and table 6 for C_s site.

^bMorrison and Leavitt (1979) [5].

^cChang et al (1982) [8] (C_2 site).

Table 12. Predicted energy levels for Ce³⁺ in Ca₅(PO₄)₃F, C₃ site. B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm ⁻¹)	Free ion mixture (%)
1	$\Gamma_{4,5}$	$2F_{5/2}$	0	$97.52\ 2F_{5/2} + 2.48\ 2F_{7/2}$
2	$\Gamma_{4,5}$	250	573.8	$93.34\ 2F_{5/2} + 6.66\ 2F_{7/2}$
3	$2\Gamma_6$	—	1074.1	$96.86\ 2F_{5/2} + 3.14\ 2F_{7/2}$
4	$\Gamma_{4,5}$	$2F_{7/2}$	2272.0	$97.75\ 2F_{7/2} + 2.25\ 2F_{5/2}$
5	$\Gamma_{4,5}$	2550	2771.5	$97.60\ 2F_{7/2} + 2.40\ 2F_{5/2}$
6	$2\Gamma_6$	—	3532.0	$96.86\ 2F_{7/2} + 3.14\ 2F_{5/2}$
7	$\Gamma_{4,5}$	—	3559.9	$95.51\ 2F_{7/2} + 49\ 2F_{5/2}$

^aIrreducible representations of C₃ double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.

^bAqueous centroids (cm⁻¹).

Table 13. Predicted energy levels for Pr³⁺ in Ca₅(PO₄)₃F, C₃ site. B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm ⁻¹)	Free ion mixture (%)
1	Γ_1	$3H_4$	0	$98.44\ 3H_4 + 0.69\ 3F_3 + 0.63\ 3H_5$
2	$\Gamma_{2,3}$	245	109	$96.47\ 3H_4 + 2.05\ 3H_5 + 1.15\ 3F_2$
3	Γ_1		167	$99.25\ 3H_4 + 0.23\ 3F_3 + 0.19\ 3F_4$
4	$\Gamma_{2,3}$		254	$98.26\ 3H_4 + 1.17\ 3H_5 + 0.24\ 3F_2$
5	$\Gamma_{2,3}$		739	$95.94\ 3H_4 + 3.59\ 3H_5 + 0.25\ 3F_2$
6	Γ_1		1114	$98.45\ 3H_4 + 0.86\ 3H_5 + 0.45\ 3F_3$
7	$\Gamma_{2,3}$	$3H_5$	2193	$96.77\ 3H_5 + 1.24\ 3H_4 + 0.69\ 3H_6$
8	Γ_1	2323	2200	$97.50\ 3H_5 + 1.07\ 3F_3 + 0.57\ 3H_4$
9	Γ_1		2258	$95.80\ 3H_5 + 1.88\ 3H_6 + 1.10\ 3F_3$
10	$\Gamma_{2,3}$		2289	$98.23\ 3H_5 + 0.69\ 3H_6 + 0.33\ 3F_2$
11	$\Gamma_{2,3}$		2509	$92.33\ 3H_5 + 3.00\ 3H_6 + 2.63\ 3H_4$
12	$\Gamma_{2,3}$		2928	$93.88\ 3H_5 + 2.97\ 3H_4 + 1.58\ 3H_6$
13	Γ_1		3089	$98.55\ 3H_5 + 0.89\ 3H_6 + 0.25\ 3F_3$
14	$\Gamma_{2,3}$	$3H_6$	4184	$93.75\ 3H_6 + 3.10\ 3F_4 + 1.58\ 3H_5$
15	Γ_1	4496	4230	$95.23\ 3H_6 + 1.61\ 3F_3 + 1.55\ 3H_5$
16	Γ_1		4354	$96.64\ 3H_6 + 1.51\ 3F_2 + 1.19\ 3F_4$
17	$\Gamma_{2,3}$		4441	$96.23\ 3H_6 + 2.05\ 3F_2 + 0.98\ 3F_3$
18	Γ_1		4533	$96.29\ 3H_6 + 1.61\ 3H_5 + 1.51\ 3F_3$
19	Γ_1		4578	$96.48\ 3H_6 + 1.89\ 3F_3 + 1.05\ 3H_5$
20	$\Gamma_{2,3}$		4894	$88.71\ 3H_6 + 7.40\ 3F_2 + 3.29\ 3H_5$
21	$\Gamma_{2,3}$		5196	$83.31\ 3H_6 + 13.85\ 3F_2 + 1.37\ 3F_4$
22	Γ_1	$3F_2$	5256	$60.34\ 3F_2 + 37.03\ 3H_6 + 1.49\ 3F_4$
23	$\Gamma_{2,3}$	5149	5337	$87.55\ 3F_2 + 10.60\ 3H_6 + 0.88\ 3H_5$
24	Γ_1	$3F_3$	5396	$58.13\ 3H_6 + 36.57\ 3F_2 + 4.03\ 3F_3$
25	$\Gamma_{2,3}$	6540	5680	$78.14\ 3F_2 + 11.21\ 3H_6 + 6.58\ 3F_3$
26	Γ_1	$3F_4$	6611	$89.27\ 3F_3 + 9.76\ 3F_4 + 0.83\ 3H_6$
27	$\Gamma_{2,3}$	6973	6725	$92.97\ 3F_3 + 3.17\ 3F_4 + 1.99\ 3F_2$
28	Γ_1		6762	$69.01\ 3F_4 + 27.32\ 3F_3 + 1.44\ 1G_4$
29	Γ_1		6819	$54.19\ 3F_3 + 43.19\ 3F_4 + 1.58\ 3H_6$
30	$\Gamma_{2,3}$		6868	$92.78\ 3F_3 + 2.46\ 3H_6 + 2.24\ 3F_2$
31	$\Gamma_{2,3}$		7135	$97.90\ 3F_4 + 0.65\ 3H_6 + 0.48\ 3F_2$
32	Γ_1		7189	$68.99\ 3F_4 + 26.80\ 3F_3 + 2.67\ 3H_6$
33	$\Gamma_{2,3}$		7219	$95.78\ 3F_4 + 2.48\ 3F_3 + 0.93\ 3H_6$
34	Γ_1		7249	$55.00\ 3F_3 + 39.15\ 3F_4 + 3.40\ 3H_6$
35	Γ_1		7408	$58.80\ 3F_4 + 32.86\ 3F_3 + 5.56\ 3H_6$
36	$\Gamma_{2,3}$		7619	$93.02\ 3F_4 + 4.11\ 3H_6 + 1.07\ 3F_3$

Table 13 (cont'd).
Predicted energy
levels for Pr^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S, L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
37	Γ_1	1G_4	9560	$95.75 ^1G_4 + 3.09 ^3F_4 + 0.56 ^3H_6$
38	Γ_1	9885	9723	$97.92 ^1G_4 + 1.11 ^3F_4 + 0.50 ^3H_6$
39	$\Gamma_{2,3}$		10039	$98.87 ^1G_4 + 0.43 ^3F_4 + 0.30 ^3H_6$
40	$\Gamma_{2,3}$		10103	$99.33 ^1G_4 + 0.14 ^3H_6 + 0.13 ^1I_6$
41	Γ_1		10223	$99.42 ^1G_4 + 0.18 ^1I_6 + 0.13 ^3F_4$
42	$\Gamma_{2,3}$		10645	$98.71 ^1G_4 + 0.53 ^3F_4 + 0.32 ^3H_6$
43	Γ_1	1D_2	16328	$98.12 ^1D_2 + 1.52 ^1I_6 + 0.16 ^3P_2$
44	$\Gamma_{2,3}$	16840	17079	$99.18 ^1D_2 + 0.51 ^1I_6 + 0.09 ^1G_4$
45	$\Gamma_{2,3}$		17323	$98.31 ^1D_2 + 1.36 ^1I_6 + 0.14 ^1G_4$
46	Γ_1	3P_0	20425	$99.97 ^1I_6 + 0.02 ^1G_4$
47	Γ_1	20706	20444	$99.33 ^1I_6 + 0.52 ^1D_2 + 0.11 ^3P_2$
48	Γ_1	3P_1	20897	$94.80 ^3P_0 + 4.34 ^3P_2 + 0.52 ^1I_6$
49	$\Gamma_{2,3}$	21330	21384	$90.11 ^3P_1 + 6.45 ^3P_2 + 2.95 ^1I_6$
50	$\Gamma_{2,3}$	1I_6	21490	$97.05 ^1I_6 + 2.60 ^3P_1 + 0.20 ^1D_2$
51	Γ_1	21500	21789	$96.46 ^1I_6 + 1.88 ^3P_2 + 0.68 ^3P_0$
52	$\Gamma_{2,3}$		21810	$99.17 ^1I_6 + 0.37 ^3P_2 + 0.31 ^1D_2$
53	Γ_1		21837	$99.87 ^3P_1 + 0.07 ^3H_5 + 0.03 ^1I_6$
54	$\Gamma_{2,3}$		22168	$97.74 ^1I_6 + 1.30 ^3P_2 + 0.45 ^1D_2$
55	$\Gamma_{2,3}$		22265	$92.16 ^1I_6 + 5.80 ^3P_2 + 1.12 ^3P_1$
56	Γ_1		22270	$98.27 ^1I_6 + 1.10 ^3P_2 + 0.24 ^1G_4$
57	Γ_1		22354	$83.70 ^1I_6 + 14.27 ^3P_2 + 1.35 ^3P_0$
58	Γ_1	3P_2	22622	$77.80 ^3P_2 + 19.24 ^1I_6 + 2.67 ^3P_0$
59	$\Gamma_{2,3}$	22535	22840	$87.98 ^3P_2 + 6.46 ^1I_6 + 5.20 ^3P_1$
60	$\Gamma_{2,3}$		23056	$97.62 ^3P_2 + 2.10 ^1I_6 + 0.11 ^3P_1$
61	Γ_1	1S_0	47169	$99.86 ^1S_0 + 0.06 ^1I_6 + 0.03 ^1D_2$
		46901		

^aIrreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.

^bAqueous centroids (cm^{-1}).

Table 14. Predicted
energy levels for Nd^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S, L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
1	$\Gamma_{4,5}$	$^4I_{9/2}$	0	$98.44 ^4I_{9/2} + 1.38 ^4I_{11/2} + 0.13 ^4I_{13/2}$
2	$2\Gamma_6$	130	25	$97.83 ^4I_{9/2} + 1.80 ^4I_{11/2} + 0.28 ^4I_{13/2}$
3	$\Gamma_{4,5}$		335	$97.23 ^4I_{9/2} + 2.62 ^4I_{11/2} + 0.05 ^4G_{5/2}$
4	$\Gamma_{4,5}$		530	$99.12 ^4I_{9/2} + 0.53 ^4I_{11/2} + 0.17 ^4I_{13/2}$
5	$2\Gamma_6$		658	$97.75 ^4I_{9/2} + 2.06 ^4I_{11/2} + 0.08 ^4I_{13/2}$
6	$2\Gamma_6$	$^4I_{11/2}$	2060	$96.95 ^4I_{11/2} + 1.58 ^4I_{9/2} + 1.34 ^4I_{13/2}$
7	$\Gamma_{4,5}$	2006	2142	$97.09 ^4I_{11/2} + 2.34 ^4I_{13/2} + 0.24 ^4I_{9/2}$
8	$\Gamma_{4,5}$		2174	$95.48 ^4I_{11/2} + 2.22 ^4I_{9/2} + 2.16 ^4I_{13/2}$
9	$\Gamma_{4,5}$		2376	$97.27 ^4I_{11/2} + 1.59 ^4I_{9/2} + 1.03 ^4I_{13/2}$
10	$\Gamma_{4,5}$		2403	$98.94 ^4I_{11/2} + 0.41 ^4I_{9/2} + 0.33 ^4I_{13/2}$
11	$2\Gamma_6$		2415	$96.68 ^4I_{11/2} + 2.28 ^4I_{9/2} + 0.86 ^4I_{13/2}$
12	$\Gamma_{4,5}$	$^4I_{13/2}$	4015	$97.45 ^4I_{13/2} + 1.49 ^4I_{11/2} + 0.98 ^4I_{15/2}$
13	$2\Gamma_6$	4004	4104	$96.39 ^4I_{13/2} + 1.79 ^4I_{15/2} + 1.51 ^4I_{11/2}$
14	$\Gamma_{4,5}$		4121	$96.90 ^4I_{13/2} + 2.48 ^4I_{15/2} + 0.46 ^4I_{11/2}$
15	$\Gamma_{4,5}$		4385	$97.53 ^4I_{13/2} + 1.58 ^4I_{11/2} + 0.55 ^4I_{15/2}$
16	$2\Gamma_6$		4404	$98.04 ^4I_{13/2} + 0.98 ^4I_{15/2} + 0.68 ^4I_{11/2}$
17	$\Gamma_{4,5}$		4408	$97.64 ^4I_{13/2} + 1.06 ^4I_{15/2} + 1.05 ^4I_{11/2}$
18	$\Gamma_{4,5}$		4436	$98.01 ^4I_{13/2} + 1.18 ^4I_{11/2} + 0.68 ^4I_{15/2}$

Table 14 (cont'd).
Predicted energy
levels for Nd³⁺ in
Ca₅(PO₄)₃F, C₃ site.
B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm ⁻¹)	Free ion mixture (%)
19	$\Gamma_{4,5}$	$4I_{15/2}$	5890	97.87 $4I_{15/2}$ + 1.99 $4I_{13/2}$ + 0.04 $4F_{9/2}$
20	$\Gamma_{4,5}$	6080	6059	98.64 $4I_{15/2}$ + 1.10 $4I_{13/2}$ + 0.17 $4I_{11/2}$
21	$2\Gamma_6$		6144	99.01 $4I_{15/2}$ + 0.83 $4I_{13/2}$ + 0.04 $4F_{9/2}$
22	$\Gamma_{4,5}$		6377	98.63 $4I_{15/2}$ + 1.08 $4I_{13/2}$ + 0.11 $4I_{11/2}$
23	$2\Gamma_6$		6497	99.25 $4I_{15/2}$ + 0.39 $4I_{13/2}$ + 0.09 $4F_{9/2}$
24	$\Gamma_{4,5}$		6544	99.04 $4I_{15/2}$ + 0.52 $4I_{13/2}$ + 0.13 $4F_{9/2}$
25	$\Gamma_{4,5}$		6675	98.67 $4I_{15/2}$ + 1.02 $4I_{13/2}$ + 0.08 $4F_{9/2}$
26	$2\Gamma_6$		6732	98.32 $4I_{15/2}$ + 1.51 $4I_{13/2}$ + 0.06 $4I_{11/2}$
27	$\Gamma_{4,5}$	$4F_{3/2}$	11678	97.83 $4F_{3/2}$ + 0.63 $4F_{5/2}$ + 0.56 $2H_{9/2}$
28	$2\Gamma_6$	11526	11826	94.37 $4F_{3/2}$ + 3.69 $4F_{5/2}$ + 0.93 $4F_{7/2}$
29	$\Gamma_{4,5}$	$4F_{5/2}$	12670	86.44 $4F_{5/2}$ + 11.44 $2H_{9/2}$ + 1.02 $4F_{7/2}$
30	$\Gamma_{4,5}$	12573	12800	56.77 $4F_{5/2}$ + 37.86 $2H_{9/2}$ + 4.03 $4F_{7/2}$
31	$2\Gamma_6$	$2H_{9/2}$	12831	87.91 $2H_{9/2}$ + 9.92 $4F_{5/2}$ + 0.98 $4F_{3/2}$
32	$\Gamma_{4,5}$	12738	12912	63.42 $2H_{9/2}$ + 34.89 $4F_{5/2}$ + 0.95 $4F_{7/2}$
33	$2\Gamma_6$		12943	83.94 $4F_{5/2}$ + 12.03 $2H_{9/2}$ + 3.30 $4F_{3/2}$
34	$\Gamma_{4,5}$		13039	85.76 $2H_{9/2}$ + 12.40 $4F_{5/2}$ + 1.17 $4F_{7/2}$
35	$2\Gamma_6$		13147	98.06 $2H_{9/2}$ + 1.29 $4F_{5/2}$ + 0.23 $4F_{9/2}$
36	$\Gamma_{4,5}$		13174	98.22 $2H_{9/2}$ + 0.87 $4F_{7/2}$ + 0.40 $4F_{5/2}$
37	$\Gamma_{4,5}$		13657	92.59 $4F_{7/2}$ + 2.80 $4F_{5/2}$ + 1.79 $4S_{3/2}$
38	$\Gamma_{4,5}$	$4S_{3/2}$	13711	96.19 $4S_{3/2}$ + 2.60 $4F_{7/2}$ + 0.43 $4G_{5/2}$
39	$2\Gamma_6$	13459	13737	94.92 $4S_{3/2}$ + 4.12 $4F_{7/2}$ + 0.20 $4G_{5/2}$
40	$2\Gamma_6$	$4F_{7/2}$	13872	92.28 $4F_{7/2}$ + 4.33 $4S_{3/2}$ + 0.93 $2H_{9/2}$
41	$\Gamma_{4,5}$	13564	13884	95.10 $4F_{7/2}$ + 2.24 $4F_{5/2}$ + 1.12 $4F_{9/2}$
42	$\Gamma_{4,5}$		13982	94.68 $4F_{7/2}$ + 3.29 $4F_{9/2}$ + 1.23 $4F_{5/2}$
43	$\Gamma_{4,5}$	$4F_{9/2}$	15018	97.36 $4F_{9/2}$ + 0.89 $2H_{11/2}$ + 0.53 $4F_{7/2}$
44	$\Gamma_{4,5}$	14854	15082	95.39 $4F_{9/2}$ + 3.08 $4F_{7/2}$ + 0.71 $2H_{11/2}$
45	$2\Gamma_6$		15086	98.04 $4F_{9/2}$ + 0.71 $4F_{7/2}$ + 0.41 $2H_{11/2}$
46	$\Gamma_{4,5}$		15166	97.49 $4F_{9/2}$ + 1.46 $4F_{7/2}$ + 0.32 $2G_{7/2}$
47	$2\Gamma_6$		15380	99.07 $4F_{9/2}$ + 0.31 $2G_{7/2}$ + 0.21 $2H_{9/2}$
48	$\Gamma_{4,5}$	$2H_{11/2}$	16263	98.22 $2H_{11/2}$ + 1.15 $2G_{7/2}$ + 0.15 $4F_{7/2}$
49	$2\Gamma_6$	16043	16282	98.78 $2H_{11/2}$ + 0.81 $2G_{7/2}$ + 0.11 $4F_{9/2}$
50	$\Gamma_{4,5}$		16308	97.59 $2H_{11/2}$ + 1.76 $2G_{7/2}$ + 0.33 $4F_{9/2}$
51	$2\Gamma_6$		16319	98.63 $2H_{11/2}$ + 0.50 $2G_{7/2}$ + 0.46 $4F_{9/2}$
52	$\Gamma_{4,5}$		16350	98.30 $2H_{11/2}$ + 0.88 $4F_{9/2}$ + 0.33 $2H_{9/2}$
53	$\Gamma_{4,5}$		16404	98.99 $2H_{11/2}$ + 0.46 $4F_{9/2}$ + 0.35 $2G_{7/2}$
54	$\Gamma_{4,5}$	$4G_{5/2}$	17215	83.80 $4G_{5/2}$ + 14.59 $2G_{7/2}$ + 0.37 $2H_{11/2}$
55	$\Gamma_{4,5}$	17167	17379	73.71 $4G_{5/2}$ + 25.12 $2G_{7/2}$ + 0.50 $2H_{11/2}$
56	$2\Gamma_6$	$2G_{7/2}$	17490	64.48 $2G_{7/2}$ + 33.67 $4G_{5/2}$ + 0.96 $2H_{11/2}$
57	$\Gamma_{4,5}$	17334	17674	96.68 $2G_{7/2}$ + 1.56 $4G_{5/2}$ + 1.06 $2H_{11/2}$
58	$\Gamma_{4,5}$		17734	84.89 $2G_{7/2}$ + 13.79 $4G_{5/2}$ + 0.51 $2H_{11/2}$
59	$\Gamma_{4,5}$		17799	72.81 $2G_{7/2}$ + 24.91 $4G_{5/2}$ + 1.10 $2H_{11/2}$
60	$2\Gamma_6$		17815	65.04 $4G_{5/2}$ + 33.45 $2G_{7/2}$ + 0.49 $2H_{11/2}$

^aIrreducible representations of C₃ double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.

^bAqueous centroids (cm⁻¹).

Table 15. Predicted energy levels for Pm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site. B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm ⁻¹)	Free ion mixture (%)
1	$\Gamma_{2,3}$	5I_4	0	$98.57 ^5I_4 + 1.14 ^5I_5 + 0.22 ^5I_6$
2	Γ_1	99	122	$99.19 ^5I_4 + 0.63 ^5I_5 + 0.08 ^5I_6$
3	$\Gamma_{2,3}$		143	$96.77 ^5I_4 + 2.88 ^5I_5 + 0.27 ^5I_6$
4	$\Gamma_{2,3}$		320	$97.47 ^5I_4 + 1.86 ^5I_5 + 0.57 ^5I_6$
5	Γ_1		368	$93.90 ^5I_4 + 5.70 ^5I_5 + 0.30 ^5I_6$
6	Γ_1		547	$97.57 ^5I_4 + 1.82 ^5I_5 + 0.54 ^5I_6$
7	Γ_1	5I_5	1533	$99.55 ^5I_5 + 0.14 ^5I_6 + 0.10 ^5I_7$
8	$\Gamma_{2,3}$	1577	1621	$97.20 ^5I_5 + 1.90 ^5I_6 + 0.76 ^5I_7$
9	$\Gamma_{2,3}$		1710	$98.59 ^5I_5 + 0.60 ^5I_6 + 0.46 ^5I_7$
10	$\Gamma_{2,3}$		1803	$96.94 ^5I_5 + 1.81 ^5I_6 + 0.86 ^5I_7$
11	Γ_1		1814	$94.12 ^5I_5 + 3.46 ^5I_6 + 2.26 ^5I_7$
12	$\Gamma_{2,3}$		1820	$95.21 ^5I_5 + 2.89 ^5I_6 + 1.49 ^5I_7$
13	Γ_1		1857	$92.37 ^5I_5 + 5.87 ^5I_6 + 1.30 ^5I_7$
14	Γ_1	5I_6	3154	$99.26 ^5I_6 + 0.27 ^5I_7 + 0.17 ^5I_8$
15	$\Gamma_{2,3}$	3186	3203	$98.69 ^5I_6 + 0.46 ^5I_7 + 0.42 ^5I_8$
16	$\Gamma_{2,3}$		3309	$98.29 ^5I_6 + 0.76 ^5I_7 + 0.63 ^5I_8$
17	Γ_1		3338	$96.14 ^5I_6 + 3.12 ^5I_7 + 0.36 ^5I_8$
18	Γ_1		3359	$97.09 ^5I_6 + 1.82 ^5I_7 + 0.52 ^5I_8$
19	$\Gamma_{2,3}$		3424	$96.11 ^5I_6 + 1.78 ^5I_7 + 1.59 ^5I_8$
20	$\Gamma_{2,3}$		3429	$94.94 ^5I_6 + 2.71 ^5I_7 + 1.75 ^5I_8$
21	Γ_1		3455	$97.79 ^5I_6 + 1.50 ^5I_7 + 0.62 ^5I_8$
22	Γ_1		3462	$95.98 ^5I_6 + 3.15 ^5I_7 + 0.64 ^5I_8$
23	Γ_1	5I_7	4881	$99.36 ^5I_7 + 0.23 ^5I_8 + 0.11 ^5I_9$
24	$\Gamma_{2,3}$	4876	4893	$98.68 ^5I_7 + 0.68 ^5I_8 + 0.28 ^5I_9$
25	$\Gamma_{2,3}$		4936	$97.96 ^5I_7 + 1.01 ^5I_8 + 0.67 ^5I_9$
26	Γ_1		4992	$98.20 ^5I_7 + 0.97 ^5I_8 + 0.70 ^5I_9$
27	$\Gamma_{2,3}$		5039	$95.82 ^5I_7 + 2.77 ^5I_8 + 1.21 ^5I_9$
28	Γ_1		5051	$97.04 ^5I_7 + 2.45 ^5I_8 + 0.32 ^5I_9$
29	$\Gamma_{2,3}$		5103	$96.38 ^5I_7 + 2.07 ^5I_8 + 1.33 ^5I_9$
30	$\Gamma_{2,3}$		5141	$93.94 ^5I_7 + 4.28 ^5I_8 + 1.24 ^5I_9$
31	Γ_1		5217	$96.98 ^5I_7 + 1.52 ^5I_8 + 1.40 ^5I_9$
32	Γ_1		5219	$97.16 ^5I_7 + 1.53 ^5I_8 + 1.25 ^5I_9$
33	Γ_1	5I_8	6529	$98.68 ^5I_8 + 1.05 ^5I_9 + 0.11 ^5I_{10}$
34	$\Gamma_{2,3}$	6611	6548	$98.25 ^5I_8 + 1.47 ^5I_9 + 0.16 ^5I_{10}$
35	$\Gamma_{2,3}$		6590	$96.63 ^5I_8 + 3.26 ^5I_9 + 0.03 ^5F_4$
36	Γ_1		6599	$99.25 ^5I_8 + 0.40 ^5I_9 + 0.14 ^5I_{10}$
37	$\Gamma_{2,3}$		6633	$98.63 ^5I_8 + 1.04 ^5I_9 + 0.16 ^5I_{10}$
38	Γ_1		6795	$98.69 ^5I_8 + 0.92 ^5I_9 + 0.30 ^5I_{10}$
39	$\Gamma_{2,3}$		6797	$97.28 ^5I_8 + 2.50 ^5I_9 + 0.11 ^5I_{10}$
40	$\Gamma_{2,3}$		6986	$99.10 ^5I_8 + 0.74 ^5I_9 + 0.04 ^5I_{10}$
41	Γ_1		7083	$99.04 ^5I_8 + 0.60 ^5I_9 + 0.28 ^5I_{10}$
42	Γ_1		7104	$98.97 ^5I_8 + 0.72 ^5I_9 + 0.21 ^5I_{10}$
43	$\Gamma_{2,3}$		7202	$98.74 ^5I_8 + 1.16 ^5I_9 + 0.03 ^5F_5$
44	$\Gamma_{2,3}$	5F_1	12460	$89.51 ^5F_1 + 8.57 ^5F_2 + 1.56 ^5F_3$
45	Γ_1	12397	12671	$98.86 ^5F_1 + 0.73 ^5F_3 + 0.20 ^5F_5$
46	$\Gamma_{2,3}$	5F_2	12872	$93.52 ^5F_2 + 3.34 ^5F_1 + 2.11 ^5F_3$
47	$\Gamma_{2,3}$	12811	12979	$92.47 ^5F_2 + 5.57 ^5F_1 + 1.01 ^5F_3$
48	Γ_1		13215	$99.53 ^5F_2 + 0.16 ^5F_4 + 0.13 ^5F_5$

Table 15 (cont'd).
Predicted energy
levels for Pm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
49	Γ_1	5F_3	13699	$93.55 ^5F_3 + 5.73 ^5F_4 + 0.44 ^5F_5$
50	$\Gamma_{2,3}$	13651	13720	$96.27 ^5F_3 + 2.74 ^5F_2 + 0.39 ^5F_5$
51	Γ_1		13780	$95.55 ^5F_3 + 3.74 ^5F_4 + 0.32 ^5F_1$
52	$\Gamma_{2,3}$		13941	$96.75 ^5F_3 + 1.06 ^5F_1 + 1.03 ^5F_4$
53	Γ_1		13956	$97.36 ^5F_3 + 2.14 ^5F_4 + 0.25 ^5F_1$
54	$\Gamma_{2,3}$	5S_2	14512	$99.51 ^5S_2 + 0.34 ^5F_4 + 0.04 ^5I_8$
55	Γ_1	14337	14516	$99.81 ^5S_2 + 0.06 ^5F_4 + 0.05 ^5I_8$
56	$\Gamma_{2,3}$		14520	$99.58 ^5S_2 + 0.25 ^5F_4 + 0.04 ^5F_3$
57	$\Gamma_{2,3}$	5F_4	14626	$96.50 ^5F_4 + 2.63 ^5F_5 + 0.53 ^5F_3$
58	$\Gamma_{2,3}$	14561	14728	$97.89 ^5F_4 + 0.71 ^5F_2 + 0.51 ^5F_5$
59	Γ_1		14770	$97.60 ^5F_4 + 1.48 ^5F_3 + 0.46 ^5F_5$
60	$\Gamma_{2,3}$		14798	$97.56 ^5F_4 + 0.92 ^5F_5 + 0.71 ^5F_3$
61	Γ_1		14809	$92.42 ^5F_4 + 6.44 ^5F_3 + 0.91 ^5F_5$
62	Γ_1		14887	$95.80 ^5F_4 + 3.83 ^5F_3 + 0.11 ^5F_5$
63	$\Gamma_{2,3}$	5F_5	15771	$99.05 ^5F_5 + 0.67 ^3K_6 + 0.14 ^5F_4$
64	$\Gamma_{2,3}$	15862	16006	$93.25 ^3K_6 + 6.60 ^5F_5 + 0.11 ^5F_4$
65	Γ_1	3K_6	16010	$57.52 ^5F_5 + 41.71 ^3K_6 + 0.50 ^5F_4$
66	$\Gamma_{2,3}$	15874	16012	$94.66 ^3K_6 + 5.20 ^5F_5 + 0.11 ^5F_4$
67	Γ_1		16022	$99.24 ^3K_6 + 0.69 ^5F_5 + 0.06 ^5F_4$
68	Γ_1		16029	$61.17 ^3K_6 + 38.51 ^5F_5 + 0.17 ^5F_4$
69	$\Gamma_{2,3}$		16041	$74.51 ^5F_5 + 24.16 ^3K_6 + 1.01 ^5F_4$
70	Γ_1		16042	$97.85 ^3K_6 + 2.02 ^5F_5 + 0.08 ^5F_4$
71	Γ_1		16042	$96.69 ^3K_6 + 3.22 ^5F_5 + 0.06 ^5F_4$
72	$\Gamma_{2,3}$		16067	$94.58 ^3K_6 + 5.33 ^5F_5 + 0.05 ^5F_4$
73	Γ_1		16096	$99.12 ^3K_6 + 0.83 ^5F_5 + 0.04 ^5F_4$
74	$\Gamma_{2,3}$		16097	$82.70 ^3K_6 + 16.87 ^5F_5 + 0.36 ^5F_4$
75	$\Gamma_{2,3}$		16154	$92.96 ^5F_5 + 6.02 ^3K_6 + 0.44 ^5F_3$
76	$\Gamma_{2,3}$		16178	$94.01 ^5F_5 + 3.74 ^3K_6 + 1.95 ^5F_4$
77	Γ_1		16200	$96.88 ^5F_5 + 2.01 ^3K_6 + 0.65 ^5F_4$
78	Γ_1		16218	$97.33 ^5F_5 + 1.88 ^3K_6 + 0.36 ^5F_4$

^aIrreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.

^bAqueous centroids (cm^{-1}).

Table 16. Predicted
energy levels for
 Sm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$,
 C_3 site. B_{nm} from
table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
1	$\Gamma_{4,5}$	$^6H_{5/2}$	0	$95.35 ^6H_{5/2} + 3.20 ^6H_{7/2} + 1.00 ^6H_{9/2}$
2	$^2\Gamma_6$	46	279	$88.50 ^6H_{5/2} + 10.12 ^6H_{7/2} + 0.83 ^6H_{9/2}$
3	$\Gamma_{4,5}$		570	$97.98 ^6H_{5/2} + 1.27 ^6H_{7/2} + 0.43 ^6H_{9/2}$
4	$^2\Gamma_6$	$^6H_{7/2}$	1227	$85.60 ^6H_{7/2} + 10.69 ^6H_{5/2} + 3.04 ^6H_{9/2}$
5	$\Gamma_{4,5}$	1084	1234	$92.82 ^6H_{7/2} + 3.42 ^6H_{5/2} + 2.21 ^6H_{9/2}$
6	$\Gamma_{4,5}$		1433	$94.34 ^6H_{7/2} + 4.03 ^6H_{9/2} + 0.84 ^6H_{5/2}$
7	$\Gamma_{4,5}$		1630	$98.28 ^6H_{7/2} + 0.88 ^6H_{9/2} + 0.30 ^6H_{5/2}$
8	$\Gamma_{4,5}$	$^6H_{9/2}$	2411	$89.65 ^6H_{9/2} + 5.91 ^6H_{7/2} + 2.86 ^6H_{11/2}$
9	$^2\Gamma_6$	2299	2456	$93.27 ^6H_{9/2} + 3.42 ^6H_{7/2} + 2.57 ^6H_{11/2}$
10	$\Gamma_{4,5}$		2562	$94.72 ^6H_{9/2} + 1.55 ^6H_{11/2} + 1.29 ^6H_{7/2}$
11	$\Gamma_{4,5}$		2694	$96.20 ^6H_{9/2} + 2.54 ^6H_{11/2} + 0.48 ^6H_{13/2}$
12	$^2\Gamma_6$		2858	$99.04 ^6H_{9/2} + 0.34 ^6H_{11/2} + 0.14 ^6H_{7/2}$

Table 16 (cont'd).
Predicted energy
levels for Sm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm^{-1})	Free ion mixture (%)
13	$\Gamma_{4,5}$	${}^6H_{11/2}$	3729	$90.82 {}^6H_{11/2} + 4.56 {}^6H_{9/2} + 2.80 {}^6H_{13/2}$
14	$2\Gamma_6$	3638	3763	$92.92 {}^6H_{11/2} + 2.91 {}^6H_{13/2} + 2.37 {}^6H_{9/2}$
15	$\Gamma_{4,5}$		3836	$94.96 {}^6H_{11/2} + 1.91 {}^6H_{9/2} + 1.67 {}^6H_{13/2}$
16	$\Gamma_{4,5}$		3932	$94.60 {}^6H_{11/2} + 2.69 {}^6H_{13/2} + 1.39 {}^6H_{9/2}$
17	$2\Gamma_6$		4125	$98.33 {}^6H_{11/2} + 0.45 {}^6F_{9/2} + 0.44 {}^6H_{13/2}$
18	$\Gamma_{4,5}$		4203	$99.25 {}^6H_{11/2} + 0.20 {}^6H_{13/2} + 0.14 {}^6F_{11/2}$
19	$2\Gamma_6$	${}^6H_{13/2}$	5100	$90.06 {}^6H_{13/2} + 4.58 {}^6H_{15/2} + 2.39 {}^6H_{11/2}$
20	$\Gamma_{4,5}$	5060	5138	$92.55 {}^6H_{13/2} + 2.89 {}^6H_{15/2} + 2.35 {}^6H_{11/2}$
21	$\Gamma_{4,5}$		5165	$92.52 {}^6H_{13/2} + 2.65 {}^6H_{11/2} + 2.63 {}^6H_{15/2}$
22	$\Gamma_{4,5}$		5317	$94.36 {}^6H_{13/2} + 2.83 {}^6H_{11/2} + 1.75 {}^6H_{15/2}$
23	$2\Gamma_6$		5500	$98.24 {}^6H_{13/2} + 0.51 {}^6H_{11/2} + 0.50 {}^6H_{15/2}$
24	$\Gamma_{4,5}$		5603	$97.75 {}^6H_{13/2} + 0.64 {}^6F_{11/2} + 0.48 {}^6F_{5/2}$
25	$\Gamma_{4,5}$		5610	$98.74 {}^6H_{13/2} + 0.27 {}^6F_{11/2} + 0.25 {}^6F_{5/2}$
26	$\Gamma_{4,5}$	${}^6F_{15/2}$	6342	$95.00 {}^6H_{15/2} + 2.13 {}^6H_{13/2} + 0.67 {}^6H_{11/2}$
27	$2\Gamma_6$	6422	6499	$92.01 {}^6H_{15/2} + 4.00 {}^6H_{13/2} + 1.56 {}^6F_{5/2}$
28	$\Gamma_{4,5}$	${}^6H_{15/2}$	6696	$91.22 {}^6H_{15/2} + 2.97 {}^6H_{13/2} + 2.22 {}^6F_{5/2}$
29	$\Gamma_{4,5}$	6531	6798	$92.24 {}^6F_{1/2} + 2.35 {}^6F_{3/2} + 2.15 {}^6H_{15/2}$
30	$\Gamma_{4,5}$	${}^6F_{3/2}$	6890	$84.70 {}^6H_{15/2} + 7.35 {}^6F_{3/2} + 2.38 {}^6F_{1/2}$
31	$2\Gamma_6$	6666	6962	$72.51 {}^6H_{15/2} + 24.49 {}^6F_{3/2} + 1.42 {}^6F_{9/2}$
32	$\Gamma_{4,5}$		7032	$52.60 {}^6F_{3/2} + 40.71 {}^6H_{15/2} + 3.33 {}^6F_{5/2}$
33	$\Gamma_{4,5}$		7060	$95.82 {}^6H_{15/2} + 1.36 {}^6F_{3/2} + 1.10 {}^6F_{7/2}$
34	$2\Gamma_6$		7069	$77.32 {}^6H_{15/2} + 17.85 {}^6F_{3/2} + 2.92 {}^6F_{5/2}$
35	$\Gamma_{4,5}$		7071	$63.22 {}^6H_{15/2} + 30.98 {}^6F_{3/2} + 2.75 {}^6F_{5/2}$
36	$2\Gamma_6$		7107	$53.93 {}^6F_{3/2} + 43.44 {}^6H_{15/2} + 1.07 {}^6H_{13/2}$
37	$2\Gamma_6$	${}^6F_{5/2}$	7523	$92.97 {}^6F_{5/2} + 4.12 {}^6H_{15/2} + 0.90 {}^6H_{13/2}$
38	$\Gamma_{4,5}$	7158	7559	$94.50 {}^6F_{5/2} + 2.11 {}^6F_{3/2} + 1.90 {}^6H_{15/2}$
39	$\Gamma_{4,5}$		7611	$92.07 {}^6F_{5/2} + 5.65 {}^6H_{15/2} + 1.04 {}^6H_{13/2}$
40	$\Gamma_{4,5}$	${}^6F_{7/2}$	8324	$96.82 {}^6F_{7/2} + 1.56 {}^6H_{15/2} + 0.72 {}^6H_{13/2}$
41	$\Gamma_{4,5}$	8006	8380	$97.34 {}^6F_{7/2} + 1.63 {}^6H_{15/2} + 0.28 {}^6H_{11/2}$
42	$2\Gamma_6$		8424	$97.13 {}^6F_{7/2} + 1.11 {}^6H_{15/2} + 0.42 {}^6H_{11/2}$
43	$\Gamma_{4,5}$		8460	$95.92 {}^6F_{7/2} + 2.49 {}^6H_{15/2} + 0.69 {}^6H_{13/2}$
44	$\Gamma_{4,5}$	${}^6F_{9/2}$	9490	$98.30 {}^6F_{9/2} + 0.54 {}^6H_{13/2} + 0.54 {}^6H_{15/2}$
45	$2\Gamma_6$	9167	9508	$97.28 {}^6F_{9/2} + 1.62 {}^6H_{15/2} + 0.30 {}^6H_{11/2}$
46	$\Gamma_{4,5}$		9561	$97.20 {}^6F_{9/2} + 1.44 {}^6H_{15/2} + 0.62 {}^6H_{13/2}$
47	$2\Gamma_6$		9565	$97.87 {}^6F_{9/2} + 0.96 {}^6H_{15/2} + 0.36 {}^6F_{11/2}$
48	$\Gamma_{4,5}$		9627	$99.07 {}^6F_{9/2} + 0.36 {}^6F_{7/2} + 0.22 {}^6H_{15/2}$
49	$\Gamma_{4,5}$	${}^6F_{11/2}$	10804	$97.23 {}^6F_{11/2} + 1.59 {}^6H_{15/2} + 0.89 {}^6H_{13/2}$
50	$\Gamma_{4,5}$	10552	10915	$99.43 {}^6F_{11/2} + 0.19 {}^6F_{9/2} + 0.19 {}^6H_{15/2}$
51	$2\Gamma_6$		10917	$98.43 {}^6F_{11/2} + 0.77 {}^6H_{15/2} + 0.57 {}^6F_{9/2}$
52	$2\Gamma_6$		10969	$98.97 {}^6F_{11/2} + 0.60 {}^6H_{15/2} + 0.22 {}^6F_{9/2}$
53	$\Gamma_{4,5}$		10975	$99.39 {}^6F_{11/2} + 0.23 {}^6H_{15/2} + 0.10 {}^6F_{7/2}$
54	$\Gamma_{4,5}$		10997	$99.20 {}^6F_{11/2} + 0.44 {}^6H_{15/2} + 0.16 {}^6H_{13/2}$
55	$2\Gamma_6$	${}^4G_{5/2}$	17981	$97.84 {}^4G_{5/2} + 2.16 {}^4F_{3/2}$
56	$\Gamma_{4,5}$	17935	18177	$99.74 {}^4G_{5/2} + 0.25 {}^4F_{3/2}$
57	$\Gamma_{4,5}$		18596	$99.86 {}^4G_{5/2} + 0.14 {}^4F_{3/2}$
58	$\Gamma_{4,5}$	${}^4F_{3/2}$	19211	$99.61 {}^4F_{3/2} + 0.39 {}^4G_{5/2}$
59	$2\Gamma_6$	18899	19272	$97.84 {}^4F_{3/2} + 2.16 {}^4G_{5/2}$

^aIrreducible representations of C_3 double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.

^bAqueous centroids (cm^{-1}).

Table 17. Predicted energy levels for Eu^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site. B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm ⁻¹)	Free ion mixture (%)
1	Γ_1	7F_0	0	$95.31 {}^7F_0 + 3.64 {}^7F_2 + 0.83 {}^7F_4$
2	$\Gamma_{2,3}$	7F_1	295	$97.07 {}^7F_1 + 1.78 {}^7F_2 + 0.49 {}^7F_4$
3	Γ_1	350	574	$90.92 {}^7F_1 + 8.64 {}^7F_3 + 0.21 {}^7F_4$
4	$\Gamma_{2,3}$	7F_2	936	$95.00 {}^7F_2 + 2.56 {}^7F_3 + 0.85 {}^7F_4$
5	$\Gamma_{2,3}$	1018	1020	$91.79 {}^7F_2 + 6.40 {}^7F_3 + 0.82 {}^7F_5$
6	Γ_1		1431	$85.91 {}^7F_2 + 8.49 {}^7F_3 + 2.97 {}^7F_0$
7	Γ_1	7F_3	1826	$96.16 {}^7F_3 + 3.23 {}^7F_5 + 0.39 {}^7F_2$
8	Γ_1	1881	1870	$87.69 {}^7F_3 + 8.70 {}^7F_2 + 2.06 {}^7F_5$
9	$\Gamma_{2,3}$		1907	$87.84 {}^7F_3 + 10.17 {}^7F_4 + 0.70 {}^7F_5$
10	$\Gamma_{2,3}$		2081	$82.16 {}^7F_3 + 10.76 {}^7F_4 + 6.17 {}^7F_2$
11	Γ_1		2082	$90.22 {}^7F_3 + 8.68 {}^7F_1 + 0.48 {}^7F_5$
12	$\Gamma_{2,3}$	7F_4	2714	$84.17 {}^7F_4 + 7.54 {}^7F_3 + 6.46 {}^7F_5$
13	Γ_1	2867	2925	$95.68 {}^7F_4 + 1.74 {}^7F_3 + 0.88 {}^7F_0$
14	$\Gamma_{2,3}$		3010	$90.20 {}^7F_4 + 3.71 {}^7F_5 + 3.29 {}^7F_3$
15	$\Gamma_{2,3}$		3039	$87.20 {}^7F_4 + 7.39 {}^7F_3 + 4.49 {}^7F_5$
16	Γ_1		3168	$96.36 {}^7F_4 + 2.07 {}^7F_6 + 0.80 {}^7F_5$
17	Γ_1		3229	$93.49 {}^7F_4 + 3.56 {}^7F_5 + 2.63 {}^7F_6$
18	Γ_1	7F_5	3740	$96.85 {}^7F_5 + 1.98 {}^7F_3 + 0.87 {}^7F_4$
19	$\Gamma_{2,3}$	3928	3864	$93.66 {}^7F_5 + 3.44 {}^7F_4 + 1.58 {}^7F_6$
20	$\Gamma_{2,3}$		4016	$86.69 {}^7F_5 + 9.46 {}^7F_6 + 3.26 {}^7F_4$
21	$\Gamma_{2,3}$		4087	$90.38 {}^7F_5 + 7.34 {}^7F_6 + 1.74 {}^7F_4$
22	$\Gamma_{2,3}$		4172	$85.95 {}^7F_5 + 8.79 {}^7F_6 + 3.99 {}^7F_4$
23	Γ_1		4207	$95.68 {}^7F_5 + 2.04 {}^7F_6 + 1.60 {}^7F_3$
24	Γ_1		4319	$91.75 {}^7F_5 + 4.14 {}^7F_6 + 2.26 {}^7F_3$
25	Γ_1	7F_6	4942	$98.12 {}^7F_6 + 1.49 {}^7F_4 + 0.17 {}^7F_2$
26	$\Gamma_{2,3}$	5029	4997	$96.68 {}^7F_6 + 2.30 {}^7F_5 + 0.53 {}^7F_3$
27	Γ_1		5029	$94.29 {}^7F_6 + 3.13 {}^7F_4 + 2.08 {}^7F_5$
28	$\Gamma_{2,3}$		5046	$95.82 {}^7F_6 + 2.26 {}^7F_5 + 1.42 {}^7F_4$
29	Γ_1		5161	$95.21 {}^7F_6 + 2.93 {}^7F_5 + 1.75 {}^7F_4$
30	$\Gamma_{2,3}$		5229	$88.13 {}^7F_6 + 10.14 {}^7F_5 + 1.50 {}^7F_4$
31	$\Gamma_{2,3}$		5456	$88.47 {}^7F_6 + 11.28 {}^7F_5 + 0.14 {}^7F_4$
32	Γ_1		5732	$99.68 {}^7F_6 + 0.13 {}^7F_5 + 0.08 {}^7F_4$
33	Γ_1		5732	$99.69 {}^7F_6 + 0.12 {}^7F_5 + 0.10 {}^7F_4$
34	Γ_1	5D_0	17399	$99.85 {}^5D_0 + 0.10 {}^5L_6 + 0.05 {}^5D_2$
		17286		
35	$\Gamma_{2,3}$	5D_1	19109	$99.88 {}^5D_1 + 0.05 {}^5D_2 + 0.04 {}^5L_6$
36	Γ_1	19026	19220	$99.97 {}^5D_1 + 0.02 {}^5L_6$
37	$\Gamma_{2,3}$	5D_2	21592	$99.79 {}^5D_2 + 0.16 {}^5D_3 + 0.04 {}^5L_6$
38	Γ_1	21499	21592	$99.85 {}^5D_2 + 0.09 {}^5L_6 + 0.05 {}^5D_0$
39	$\Gamma_{2,3}$		21660	$99.88 {}^5D_2 + 0.07 {}^5L_6 + 0.05 {}^5D_1$
40	Γ_1	5D_3	24473	$99.92 {}^5D_3 + 0.07 {}^5L_6$
41	$\Gamma_{2,3}$	24390	24488	$99.81 {}^5D_3 + 0.11 {}^5D_2 + 0.07 {}^5L_6$
42	$\Gamma_{2,3}$		24500	$99.88 {}^5D_3 + 0.05 {}^5D_2 + 0.05 {}^5L_6$
43	Γ_1		24568	$99.89 {}^5D_3 + 0.10 {}^5L_6 + 0.01 {}^5D_2$
44	Γ_1		24582	$99.85 {}^5D_3 + 0.15 {}^5L_6$

Table 17 (cont'd).
Predicted energy
levels for Eu^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
45	Γ_1	$5L_6$	25199	$99.76\ 5L_6 + 0.17\ 5D_3 + 0.07\ 5D_2$
46	Γ_1	25375	25237	$99.95\ 5L_6 + 0.04\ 5D_3 + 0.01\ 5D_1$
47	Γ_1		25252	$99.93\ 5L_6 + 0.04\ 5D_3 + 0.03\ 5D_0$
48	$\Gamma_{2,3}$		25288	$99.89\ 5L_6 + 0.06\ 5D_3 + 0.04\ 5D_2$
49	$\Gamma_{2,3}$		25463	$99.96\ 5L_6 + 0.01\ 5D_2 + 0.01\ 5D_3$
50	$\Gamma_{2,3}$		25648	$99.93\ 5L_6 + 0.05\ 5D_3 + 0.02\ 5D_2$
51	Γ_1		25690	$99.92\ 5L_6 + 0.04\ 5D_3 + 0.03\ 5D_0$
52	Γ_1		25757	$99.91\ 5L_6 + 0.04\ 5D_0 + 0.04\ 5D_3$
53	$\Gamma_{2,3}$		25791	$99.95\ 5L_6 + 0.04\ 5D_2 + 0.01\ 5D_1$

^aIrreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.

^bAqueous centroids (cm^{-1}).

Table 18. Predicted
energy levels for Gd^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
1	$\Gamma_{4,5}$	$8S_{7/2}$	0	100.00 $8S_{7/2}$
2	$2\Gamma_6$	14	0.2	100.00 $8S_{7/2}$
3	$\Gamma_{4,5}$		0.6	100.00 $8S_{7/2}$
4	$\Gamma_{4,5}$		1.2	100.00 $8S_{7/2}$
5	$\Gamma_{4,5}$	$6P_{7/2}$	32096	$99.22\ 6P_{7/2} + 0.13\ 6P_{3/2} + 0.11\ 6I_{13/2}$
6	$2\Gamma_6$	32224	32116	$98.69\ 6P_{7/2} + 0.53\ 6P_{5/2} + 0.21\ 6P_{3/2}$
7	$2\Gamma_6$		32116	$98.69\ 6P_{7/2} + 0.53\ 6P_{5/2} + 0.21\ 6P_{3/2}$
8	$\Gamma_{4,5}$		32185	$98.94\ 6P_{7/2} + 0.42\ 6P_{5/2} + 0.16\ 6I_{17/2}$
9	$\Gamma_{4,5}$		32317	$99.20\ 6P_{7/2} + 0.20\ 6I_{15/2} + 0.15\ 6I_{17/2}$
10	$\Gamma_{4,5}$	$6P_{5/2}$	32663	$98.45\ 6P_{5/2} + 0.44\ 6I_{7/2} + 0.39\ 6I_{17/2}$
11	$2\Gamma_6$	32767	32673	$94.96\ 6P_{5/2} + 3.45\ 6P_{3/2} + 0.61\ 6P_{7/2}$
12	$\Gamma_{4,5}$		32803	$98.87\ 6P_{5/2} + 0.40\ 6P_{7/2} + 0.27\ 6I_{17/2}$
13	$2\Gamma_6$	$6P_{3/2}$	33235	$95.31\ 6P_{3/2} + 3.58\ 6P_{5/2} + 0.36\ 6I_{13/2}$
14	$\Gamma_{4,5}$	33303	33294	$98.46\ 6P_{3/2} + 0.33\ 6P_{5/2} + 0.32\ 6I_{15/2}$
15	$\Gamma_{4,5}$	$6I_{7/2}$	35842	$99.59\ 6I_{7/2} + 0.19\ 6P_{5/2} + 0.08\ 6I_{9/2}$
16	$2\Gamma_6$	35879	35849	$99.18\ 6I_{7/2} + 0.43\ 6I_{9/2} + 0.27\ 6P_{5/2}$
17	$\Gamma_{4,5}$		35882	$99.43\ 6I_{7/2} + 0.25\ 6P_{5/2} + 0.16\ 6I_{9/2}$
18	$\Gamma_{4,5}$		35915	$99.69\ 6I_{7/2} + 0.14\ 6P_{5/2} + 0.06\ 6I_{9/2}$
19	$\Gamma_{4,5}$	$6I_{9/2}$	36184	$98.87\ 6I_{9/2} + 0.56\ 6I_{11/2} + 0.12\ 6I_{7/2}$
20	$\Gamma_{4,5}$	36231	36201	$99.17\ 6I_{9/2} + 0.25\ 6I_{11/2} + 0.18\ 6I_{17/2}$
21	$2\Gamma_6$		36208	$98.63\ 6I_{9/2} + 0.48\ 6I_{11/2} + 0.40\ 6I_{7/2}$
22	$\Gamma_{4,5}$		36235	$98.88\ 6I_{9/2} + 0.29\ 6I_{17/2} + 0.26\ 6I_{11/2}$
23	$2\Gamma_6$		36284	$99.42\ 6I_{9/2} + 0.22\ 6I_{13/2} + 0.09\ 6I_{11/2}$
24	$\Gamma_{4,5}$	$6I_{17/2}$	36441	$92.80\ 6I_{17/2} + 4.96\ 6I_{11/2} + 1.39\ 6I_{15/2}$
25	$\Gamma_{4,5}$	36462	36442	$95.31\ 6I_{17/2} + 2.13\ 6I_{11/2} + 1.61\ 6I_{15/2}$
26	$2\Gamma_6$		36442	$96.81\ 6I_{17/2} + 1.50\ 6I_{15/2} + 1.32\ 6I_{11/2}$
27	$2\Gamma_6$		36446	$95.97\ 6I_{17/2} + 2.09\ 6I_{11/2} + 1.17\ 6I_{15/2}$
28	$\Gamma_{4,5}$		36447	$91.83\ 6I_{17/2} + 5.85\ 6I_{11/2} + 1.61\ 6I_{15/2}$
29	$\Gamma_{4,5}$		36452	$99.03\ 6I_{17/2} + 0.62\ 6I_{11/2} + 0.13\ 6I_{13/2}$
30	$\Gamma_{4,5}$		36455	$89.72\ 6I_{17/2} + 8.14\ 6I_{11/2} + 0.78\ 6I_{13/2}$
31	$2\Gamma_6$		36456	$91.64\ 6I_{17/2} + 6.87\ 6I_{11/2} + 0.76\ 6I_{13/2}$
32	$\Gamma_{4,5}$		36460	$91.98\ 6I_{17/2} + 6.59\ 6I_{11/2} + 0.48\ 6I_{13/2}$

Table 18 (cont'd).
Predicted energy
levels for Gd³⁺ in
Ca₅(PO₄)₃F, C₃ site.
B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm ⁻¹)	Free ion mixture (%)
33	$\Gamma_{4,5}$	$6I_{11/2}$	36479	$81.65\ 6I_{11/2} + 16.50\ 6I_{17/2} + 0.75\ 6I_{15/2}$
34	$\Gamma_{4,5}$	36526	36489	$89.16\ 6I_{11/2} + 8.44\ 6I_{17/2} + 1.04\ 6I_{13/2}$
35	$2\Gamma_6$		36499	$90.62\ 6I_{11/2} + 7.37\ 6I_{17/2} + 0.79\ 6I_{15/2}$
36	$2\Gamma_6$		36523	$94.28\ 6I_{11/2} + 3.31\ 6I_{17/2} + 0.93\ 6I_{13/2}$
37	$\Gamma_{4,5}$		36533	$94.74\ 6I_{11/2} + 4.16\ 6I_{17/2} + 0.44\ 6I_{15/2}$
38	$\Gamma_{4,5}$		36585	$94.46\ 6I_{11/2} + 3.43\ 6I_{15/2} + 1.37\ 6I_{13/2}$
39	$\Gamma_{4,5}$	$6I_{13/2}$	36657	$81.93\ 6I_{13/2} + 15.30\ 6I_{15/2} + 1.68\ 6I_{11/2}$
40	$2\Gamma_6$	36711	36659	$64.83\ 6I_{13/2} + 31.53\ 6I_{15/2} + 1.73\ 6I_{17/2}$
41	$\Gamma_{4,5}$	$6I_{15/2}$	36675	$74.75\ 6I_{13/2} + 21.51\ 6I_{15/2} + 2.34\ 6I_{11/2}$
42	$\Gamma_{4,5}$	36725	36692	$57.14\ 6I_{15/2} + 37.35\ 6I_{13/2} + 3.68\ 6I_{11/2}$
43	$2\Gamma_6$		36694	$59.74\ 6I_{15/2} + 38.95\ 6I_{13/2} + 0.65\ 6I_{11/2}$
44	$\Gamma_{4,5}$		36698	$67.53\ 6I_{15/2} + 31.29\ 6I_{13/2} + 0.45\ 6I_{11/2}$
45	$\Gamma_{4,5}$		36702	$75.67\ 6I_{15/2} + 23.00\ 6I_{13/2} + 0.74\ 6I_{11/2}$
46	$2\Gamma_6$		36707	$68.98\ 6I_{13/2} + 29.22\ 6I_{15/2} + 1.04\ 6I_{11/2}$
47	$\Gamma_{4,5}$		36715	$77.76\ 6I_{13/2} + 21.35\ 6I_{15/2} + 0.33\ 6I_{17/2}$
48	$\Gamma_{4,5}$		36725	$77.69\ 6I_{15/2} + 19.92\ 6I_{13/2} + 2.04\ 6I_{17/2}$
49	$2\Gamma_6$		36731	$77.10\ 6I_{15/2} + 22.26\ 6I_{13/2} + 0.28\ 6I_{11/2}$
50	$\Gamma_{4,5}$		36734	$49.57\ 6I_{13/2} + 49.23\ 6I_{15/2} + 0.75\ 6I_{17/2}$
51	$\Gamma_{4,5}$		36742	$83.78\ 6I_{15/2} + 15.30\ 6I_{13/2} + 0.32\ 6I_{17/2}$
52	$2\Gamma_6$		36782	$97.13\ 6I_{15/2} + 1.82\ 6I_{17/2} + 0.79\ 6I_{13/2}$
53	$\Gamma_{4,5}$		36790	$81.07\ 6I_{13/2} + 18.70\ 6I_{15/2} + 0.06\ 6I_{11/2}$
54	$\Gamma_{4,5}$	$6D_{9/2}$	39618	$99.24\ 6D_{9/2} + 0.27\ 6D_{7/2} + 0.18\ 6D_{1/2}$
55	$2\Gamma_6$	39779	39691	$98.73\ 6D_{9/2} + 1.09\ 6D_{7/2} + 0.05\ 6P_{5/2}$
56	$\Gamma_{4,5}$		39809	$99.06\ 6D_{9/2} + 0.74\ 6D_{7/2} + 0.06\ 6D_{5/2}$
57	$2\Gamma_6$		39828	$99.85\ 6D_{9/2} + 0.03\ 6I_{15/2} + 0.03\ 6D_{5/2}$
58	$\Gamma_{4,5}$		39882	$99.59\ 6D_{9/2} + 0.16\ 6D_{7/2} + 0.12\ 6D_{1/2}$
59	$\Gamma_{4,5}$	$6D_{1/2}$	40576	$85.99\ 6D_{1/2} + 6.73\ 6D_{7/2} + 4.32\ 6D_{3/2}$
		40621		
60	$\Gamma_{4,5}$	$6D_{7/2}$	40680	$90.88\ 6D_{7/2} + 4.65\ 6D_{3/2} + 3.69\ 6D_{5/2}$
61	$2\Gamma_6$	40713	40694	$86.07\ 6D_{7/2} + 12.11\ 6D_{3/2} + 1.07\ 6D_{9/2}$
62	$\Gamma_{4,5}$		40703	$94.59\ 6D_{7/2} + 2.47\ 6D_{1/2} + 2.20\ 6D_{3/2}$
63	$\Gamma_{4,5}$		40727	$88.07\ 6D_{7/2} + 5.04\ 6D_{1/2} + 3.64\ 6D_{5/2}$
64	$\Gamma_{4,5}$	$6D_{3/2}$	40772	$78.83\ 6D_{3/2} + 12.14\ 6D_{7/2} + 8.12\ 6D_{5/2}$
65	$2\Gamma_6$	40851	40878	$64.11\ 6D_{5/2} + 30.79\ 6D_{3/2} + 4.94\ 6D_{7/2}$
66	$2\Gamma_6$	$6D_{5/2}$	40976	$56.96\ 6D_{3/2} + 35.11\ 6D_{5/2} + 7.71\ 6D_{7/2}$
67	$\Gamma_{4,5}$	40978	41009	$89.62\ 6D_{5/2} + 4.34\ 6D_{7/2} + 3.90\ 6D_{3/2}$
68	$\Gamma_{4,5}$		41056	$91.53\ 6D_{5/2} + 3.64\ 6D_{1/2} + 3.07\ 6D_{3/2}$

^aIrreducible representations of C₃ double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.

^bAqueous centroids (cm⁻¹).

Table 19. Predicted energy levels for Tb^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site. B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm ⁻¹)	Free ion mixture (%)
1	Γ_1	7F_6	0	$99.86 {}^7F_6 + 0.04 {}^7F_4 + 0.04 {}^7F_5$
2	Γ_1	74	0	$99.86 {}^7F_6 + 0.04 {}^7F_5 + 0.03 {}^7F_4$
3	$\Gamma_{2,3}$		335	$95.82 {}^7F_6 + 4.06 {}^7F_5 + 0.08 {}^7F_4$
4	$\Gamma_{2,3}$		560	$96.69 {}^7F_6 + 2.73 {}^7F_5 + 0.46 {}^7F_4$
5	Γ_1		606	$98.64 {}^7F_6 + 0.69 {}^7F_5 + 0.61 {}^7F_4$
6	$\Gamma_{2,3}$		706	$98.73 {}^7F_6 + 0.55 {}^7F_5 + 0.48 {}^7F_4$
7	Γ_1		721	$98.43 {}^7F_6 + 0.97 {}^7F_4 + 0.37 {}^7F_5$
8	$\Gamma_{2,3}$		746	$99.05 {}^7F_6 + 0.49 {}^7F_5 + 0.23 {}^7F_3$
9	Γ_1		786	$99.29 {}^7F_6 + 0.49 {}^7F_4 + 0.10 {}^7F_2$
10	Γ_1	7F_5	2353	$95.27 {}^7F_5 + 2.02 {}^7F_4 + 1.86 {}^7F_3$
11	$\Gamma_{2,3}$	2112	2450	$92.50 {}^7F_5 + 3.78 {}^7F_4 + 3.03 {}^7F_6$
12	Γ_1		2456	$97.52 {}^7F_5 + 1.27 {}^7F_3 + 0.64 {}^7F_4$
13	$\Gamma_{2,3}$		2532	$96.27 {}^7F_5 + 2.73 {}^7F_6 + 0.58 {}^7F_4$
14	$\Gamma_{2,3}$		2594	$94.64 {}^7F_5 + 2.56 {}^7F_4 + 2.02 {}^7F_6$
15	$\Gamma_{2,3}$		2786	$96.00 {}^7F_5 + 2.60 {}^7F_4 + 0.47 {}^7F_2$
16	Γ_1		2906	$97.87 {}^7F_5 + 1.45 {}^7F_3 + 0.48 {}^7F_4$
17	Γ_1	7F_4	3622	$95.83 {}^7F_4 + 2.80 {}^7F_5 + 0.89 {}^7F_6$
18	Γ_1	3370	3684	$97.66 {}^7F_4 + 0.78 {}^7F_5 + 0.72 {}^7F_6$
19	$\Gamma_{2,3}$		3804	$86.71 {}^7F_4 + 8.84 {}^7F_3 + 3.65 {}^7F_5$
20	$\Gamma_{2,3}$		3829	$93.62 {}^7F_4 + 2.22 {}^7F_5 + 1.76 {}^7F_3$
21	Γ_1		3916	$95.92 {}^7F_4 + 1.32 {}^7F_2 + 1.24 {}^7F_3$
22	$\Gamma_{2,3}$		4097	$86.88 {}^7F_4 + 6.56 {}^7F_3 + 4.84 {}^7F_5$
23	Γ_1	7F_3	4712	$85.50 {}^7F_3 + 13.75 {}^7F_1 + 0.44 {}^7F_5$
24	$\Gamma_{2,3}$	4344	4746	$80.96 {}^7F_3 + 10.35 {}^7F_4 + 8.08 {}^7F_2$
25	$\Gamma_{2,3}$		4919	$88.39 {}^7F_3 + 9.95 {}^7F_4 + 0.70 {}^7F_2$
26	Γ_1		4941	$79.78 {}^7F_3 + 17.11 {}^7F_2 + 1.43 {}^7F_5$
27	Γ_1		4998	$96.82 {}^7F_3 + 2.37 {}^7F_5 + 0.44 {}^7F_2$
28	Γ_1	7F_2	5242	$74.42 {}^7F_2 + 17.40 {}^7F_3 + 4.65 {}^7F_0$
29	$\Gamma_{2,3}$	5028	5646	$89.62 {}^7F_2 + 8.31 {}^7F_3 + 0.96 {}^7F_1$
30	$\Gamma_{2,3}$		5716	$93.76 {}^7F_2 + 3.32 {}^7F_3 + 1.42 {}^7F_1$
31	Γ_1	7F_1	5903	$85.84 {}^7F_1 + 13.76 {}^7F_3 + 0.24 {}^7F_4$
32	$\Gamma_{2,3}$	5481	6156	$95.78 {}^7F_1 + 3.13 {}^7F_2 + 0.50 {}^7F_4$
33	Γ_1	7F_0	6307	$92.51 {}^7F_0 + 6.39 {}^7F_2 + 0.94 {}^7F_4$
		5703		
34	Γ_1	5D_4	20931	$99.75 {}^5D_4 + 0.15 {}^5G_6 + 0.05 {}^5L_{10}$
35	Γ_1	20542	20942	$99.78 {}^5D_4 + 0.12 {}^5G_6 + 0.04 {}^5L_{10}$
36	$\Gamma_{2,3}$		20970	$99.86 {}^5D_4 + 0.07 {}^5G_6 + 0.04 {}^5L_{10}$
37	$\Gamma_{2,3}$		21026	$99.76 {}^5D_4 + 0.07 {}^5G_6 + 0.06 {}^5L_{10}$
38	$\Gamma_{2,3}$		21106	$99.81 {}^5D_4 + 0.06 {}^5L_{10} + 0.05 {}^5G_5$
39	Γ_1		21127	$99.83 {}^5D_4 + 0.06 {}^5L_{10} + 0.05 {}^5G_4$
40	Γ_1	5D_3	26470	$92.51 {}^5G_6 + 3.80 {}^5D_3 + 2.39 {}^5L_{10}$
41	Γ_1	26336	26482	$95.42 {}^5G_6 + 2.51 {}^5L_{10} + 1.00 {}^5L_9$
42	$\Gamma_{2,3}$	5G_6	26732	$58.62 {}^5D_3 + 38.18 {}^5G_6 + 1.26 {}^5L_{10}$
43	Γ_1	26425	26759	$83.54 {}^5D_3 + 14.38 {}^5G_6 + 1.26 {}^5G_5$
44	$\Gamma_{2,3}$		26765	$65.09 {}^5D_3 + 32.74 {}^5G_6 + 1.06 {}^5L_{10}$
45	Γ_1		26767	$87.56 {}^5D_3 + 10.38 {}^5G_6 + 1.31 {}^5G_5$
46	Γ_1		26785	$84.32 {}^5D_3 + 14.02 {}^5G_6 + 0.92 {}^5G_5$
47	$\Gamma_{2,3}$		26836	$58.38 {}^5G_6 + 36.29 {}^5D_3 + 3.11 {}^5L_{10}$

Table 19 (cont'd).
Predicted energy
levels for Tb³⁺ in
Ca₅(PO₄)₃F, C₃ site.
B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm ⁻¹)	Free ion mixture (%)
48	$\Gamma_{2,3}$		26867	86.82 ⁵ G ₆ + 9.24 ⁵ D ₃ + 2.28 ⁵ L ₁₀
49	Γ_1		26922	90.36 ⁵ G ₆ + 6.16 ⁵ D ₃ + 2.89 ⁵ L ₁₀
50	Γ_1		26996	73.49 ⁵ G ₆ + 24.25 ⁵ D ₃ + 1.74 ⁵ L ₁₀
51	$\Gamma_{2,3}$		27050	80.13 ⁵ G ₆ + 16.40 ⁵ D ₃ + 2.54 ⁵ L ₁₀
52	$\Gamma_{2,3}$		27106	82.43 ⁵ G ₆ + 12.12 ⁵ D ₃ + 4.43 ⁵ L ₁₀
53	Γ_1		27130	87.25 ⁵ G ₆ + 7.18 ⁵ L ₁₀ + 4.40 ⁵ D ₃
54	$\Gamma_{2,3}$	⁵ L ₁₀	27332	95.93 ⁵ L ₁₀ + 2.19 ⁵ G ₆ + 0.96 ⁵ G ₅
55	Γ_1	27146	27344	97.56 ⁵ L ₁₀ + 1.94 ⁵ G ₆ + 0.25 ⁵ G ₅
56	Γ_1		27363	91.29 ⁵ L ₁₀ + 8.23 ⁵ G ₆ + 0.14 ⁵ G ₄
57	$\Gamma_{2,3}$		27389	93.87 ⁵ L ₁₀ + 4.99 ⁵ G ₆ + 0.67 ⁵ L ₉
58	$\Gamma_{2,3}$		27508	96.10 ⁵ L ₁₀ + 1.55 ⁵ G ₆ + 1.50 ⁵ L ₉
59	$\Gamma_{2,3}$		27564	95.70 ⁵ L ₁₀ + 2.70 ⁵ G ₆ + 1.24 ⁵ L ₉
60	Γ_1		27645	96.71 ⁵ L ₁₀ + 1.44 ⁵ L ₉ + 0.99 ⁵ G ₆
61	Γ_1		27689	96.23 ⁵ L ₁₀ + 2.04 ⁵ G ₆ + 1.43 ⁵ L ₉
62	Γ_1		27697	95.90 ⁵ L ₁₀ + 1.77 ⁵ G ₆ + 1.49 ⁵ L ₉
63	Γ_1		27716	96.63 ⁵ L ₁₀ + 1.75 ⁵ G ₅ + 1.16 ⁵ L ₉
64	$\Gamma_{2,3}$		27814	95.58 ⁵ L ₁₀ + 2.33 ⁵ G ₅ + 1.14 ⁵ G ₆
65	$\Gamma_{2,3}$		27909	92.71 ⁵ L ₁₀ + 5.15 ⁵ G ₅ + 1.53 ⁵ G ₆
66	Γ_1		27948	93.04 ⁵ L ₁₀ + 4.70 ⁵ G ₅ + 1.89 ⁵ G ₆
67	$\Gamma_{2,3}$		27953	97.68 ⁵ L ₁₀ + 1.86 ⁵ G ₅ + 0.37 ⁵ G ₆
68	$\Gamma_{2,3}$	⁵ G ₅	28104	93.33 ⁵ G ₅ + 1.86 ⁵ G ₆ + 1.56 ⁵ G ₄
69	$\Gamma_{2,3}$	277795	28179	79.93 ⁵ G ₅ + 11.76 ⁵ G ₄ + 5.33 ⁵ L ₁₀
70	Γ_1		28297	93.17 ⁵ G ₅ + 2.74 ⁵ L ₁₀ + 2.51 ⁵ D ₂
71	Γ_1		28320	91.88 ⁵ G ₅ + 3.94 ⁵ L ₁₀ + 2.53 ⁵ D ₂
72	$\Gamma_{2,3}$		28343	89.56 ⁵ G ₅ + 6.07 ⁵ D ₂ + 3.07 ⁵ L ₁₀
73	$\Gamma_{2,3}$		28403	88.48 ⁵ G ₅ + 6.87 ⁵ D ₂ + 2.57 ⁵ G ₄
74	Γ_1		28480	91.53 ⁵ G ₅ + 5.36 ⁵ G ₄ + 1.71 ⁵ L ₁₀
75	Γ_1	⁵ D ₂	28567	88.95 ⁵ D ₂ + 4.31 ⁵ G ₄ + 4.08 ⁵ G ₅
76	$\Gamma_{2,3}$	28150	28620	75.81 ⁵ D ₂ + 19.61 ⁵ G ₄ + 3.24 ⁵ G ₅
77	$\Gamma_{2,3}$		28698	64.04 ⁵ D ₂ + 24.07 ⁵ G ₄ + 9.27 ⁵ G ₅
78	Γ_1	⁵ G ₄	28715	70.96 ⁵ G ₄ + 27.42 ⁵ L ₉ + 0.44 ⁵ G ₆
79	Γ_1	28307	28727	57.80 ⁵ G ₄ + 35.61 ⁵ L ₉ + 3.95 ⁵ G ₅
80	$\Gamma_{2,3}$	⁵ L ₉	28757	45.16 ⁵ G ₄ + 42.06 ⁵ L ₉ + 9.91 ⁵ G ₅
81	$\Gamma_{2,3}$	28503	28814	65.89 ⁵ L ₉ + 20.94 ⁵ G ₄ + 9.12 ⁵ D ₂
82	Γ_1		28815	66.18 ⁵ L ₉ + 32.86 ⁵ G ₄ + 0.37 ⁵ L ₁₀
83	Γ_1		28827	66.85 ⁵ L ₉ + 30.56 ⁵ G ₄ + 1.46 ⁵ G ₅
84	$\Gamma_{2,3}$		28843	44.73 ⁵ G ₄ + 41.36 ⁵ L ₉ + 11.72 ⁵ D ₂
85	$\Gamma_{2,3}$		28892	50.74 ⁵ L ₉ + 39.37 ⁵ G ₄ + 4.53 ⁵ G ₅
86	$\Gamma_{2,3}$		28918	52.28 ⁵ G ₄ + 33.92 ⁵ L ₉ + 12.71 ⁵ D ₂
87	Γ_1		28919	69.33 ⁵ G ₄ + 27.70 ⁵ L ₉ + 2.26 ⁵ D ₂
88	$\Gamma_{2,3}$		28963	70.76 ⁵ L ₉ + 24.04 ⁵ G ₄ + 3.55 ⁵ D ₂
89	$\Gamma_{2,3}$		29018	94.78 ⁵ L ₉ + 2.69 ⁵ G ₄ + 1.64 ⁵ L ₁₀
90	Γ_1		29042	91.35 ⁵ L ₉ + 7.12 ⁵ G ₄ + 0.69 ⁵ L ₁₀
91	Γ_1		29104	82.25 ⁵ L ₉ + 16.14 ⁵ G ₄ + 1.17 ⁵ L ₁₀
92	$\Gamma_{2,3}$		29186	92.17 ⁵ L ₉ + 6.39 ⁵ G ₄ + 0.72 ⁵ L ₁₀
93	Γ_1		29199	97.54 ⁵ L ₉ + 1.46 ⁵ L ₁₀ + 0.64 ⁵ G ₄
94	Γ_1		29201	96.80 ⁵ L ₉ + 1.43 ⁵ L ₁₀ + 1.36 ⁵ G ₄
95	$\Gamma_{2,3}$		29253	95.96 ⁵ L ₉ + 2.89 ⁵ G ₄ + 0.40 ⁵ G ₆
96	Γ_1		29273	97.90 ⁵ L ₉ + 1.47 ⁵ G ₄ + 0.36 ⁵ G ₆

^aIrreducible representations of C₃ single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.

^bAqueous centroids (cm⁻¹).

Table 20. Predicted energy levels for Dy³⁺ in Ca₅(PO₄)₃F, C₃ site. B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm ⁻¹)	Free ion mixture (%)
1	$\Gamma_{4,5}$	${}^6H_{15/2}$	0	99.68 ${}^6H_{15/2}$ + 0.23 ${}^6F_{11/2}$ + 0.04 ${}^6H_{11/2}$
2	$2\Gamma_6$	40	1	99.84 ${}^6H_{15/2}$ + 0.12 ${}^6F_{11/2}$ + 0.01 ${}^6F_{9/2}$
3	$\Gamma_{4,5}$		32	99.93 ${}^6H_{15/2}$ + 0.02 ${}^6F_{7/2}$ + 0.01 ${}^6H_{13/2}$
4	$2\Gamma_6$		77	99.65 ${}^6H_{15/2}$ + 0.12 ${}^6H_{13/2}$ + 0.11 ${}^6F_{11/2}$
5	$\Gamma_{4,5}$		199	99.23 ${}^6H_{15/2}$ + 0.53 ${}^6H_{13/2}$ + 0.13 ${}^6F_{11/2}$
6	$\Gamma_{4,5}$		412	99.14 ${}^6H_{15/2}$ + 0.69 ${}^6H_{13/2}$ + 0.08 ${}^6F_{11/2}$
7	$2\Gamma_6$		600	99.24 ${}^6H_{15/2}$ + 0.56 ${}^6H_{13/2}$ + 0.08 ${}^6H_{11/2}$
8	$\Gamma_{4,5}$		721	99.60 ${}^6H_{15/2}$ + 0.14 ${}^6H_{11/2}$ + 0.13 ${}^6H_{13/2}$
9	$\Gamma_{4,5}$	${}^6H_{13/2}$	3443	99.01 ${}^6H_{13/2}$ + 0.75 ${}^6F_{11/2}$ + 0.13 ${}^6H_{11/2}$
10	$\Gamma_{4,5}$	3506	3481	99.80 ${}^6H_{13/2}$ + 0.12 ${}^6F_{11/2}$ + 0.02 ${}^6F_{9/2}$
11	$2\Gamma_6$		3622	99.57 ${}^6H_{13/2}$ + 0.17 ${}^6H_{11/2}$ + 0.10 ${}^6H_{15/2}$
12	$\Gamma_{4,5}$		3769	98.40 ${}^6H_{13/2}$ + 0.77 ${}^6H_{11/2}$ + 0.53 ${}^6H_{15/2}$
13	$\Gamma_{4,5}$		3858	97.42 ${}^6H_{13/2}$ + 1.32 ${}^6H_{11/2}$ + 0.73 ${}^6H_{15/2}$
14	$2\Gamma_6$		3919	97.86 ${}^6H_{13/2}$ + 0.99 ${}^6H_{11/2}$ + 0.60 ${}^6H_{15/2}$
15	$\Gamma_{4,5}$		3950	99.11 ${}^6H_{13/2}$ + 0.31 ${}^6H_{11/2}$ + 0.26 ${}^6H_{9/2}$
16	$\Gamma_{4,5}$	${}^6H_{11/2}$	5753	99.16 ${}^6H_{11/2}$ + 0.55 ${}^6F_{11/2}$ + 0.14 ${}^6H_{13/2}$
17	$2\Gamma_6$	5833	5895	97.73 ${}^6H_{11/2}$ + 0.98 ${}^6F_{11/2}$ + 0.92 ${}^6F_{9/2}$
18	$\Gamma_{4,5}$		6082	97.22 ${}^6H_{11/2}$ + 1.03 ${}^6H_{9/2}$ + 0.68 ${}^6H_{13/2}$
19	$\Gamma_{4,5}$		6160	97.41 ${}^6H_{11/2}$ + 0.82 ${}^6H_{13/2}$ + 0.80 ${}^6H_{9/2}$
20	$2\Gamma_6$		6177	96.78 ${}^6H_{11/2}$ + 1.25 ${}^6H_{9/2}$ + 1.08 ${}^6H_{13/2}$
21	$\Gamma_{4,5}$		6191	97.19 ${}^6H_{11/2}$ + 1.19 ${}^6H_{9/2}$ + 0.76 ${}^6H_{13/2}$
22	$2\Gamma_6$	${}^6H_{9/2}$	7584	83.00 ${}^6H_{9/2}$ + 15.56 ${}^6F_{11/2}$ + 1.12 ${}^6F_{9/2}$
23	$\Gamma_{4,5}$	7692	7737	66.52 ${}^6H_{9/2}$ + 31.27 ${}^6F_{11/2}$ + 1.39 ${}^6H_{11/2}$
24	$\Gamma_{4,5}$	${}^6F_{11/2}$	7826	54.57 ${}^6H_{9/2}$ + 42.45 ${}^6F_{11/2}$ + 1.45 ${}^6H_{7/2}$
25	$2\Gamma_6$	7730	7903	92.74 ${}^6F_{11/2}$ + 6.00 ${}^6H_{9/2}$ + 0.62 ${}^6H_{11/2}$
26	$\Gamma_{4,5}$	${}^6F_{9/2}$	7913	74.26 ${}^6F_{11/2}$ + 24.56 ${}^6H_{9/2}$ + 0.33 ${}^6H_{11/2}$
27	$\Gamma_{4,5}$	9087	7949	87.90 ${}^6F_{11/2}$ + 10.89 ${}^6H_{9/2}$ + 0.54 ${}^6H_{7/2}$
28	$\Gamma_{4,5}$	${}^6H_{7/2}$	8001	56.34 ${}^6H_{9/2}$ + 40.69 ${}^6F_{11/2}$ + 0.91 ${}^6H_{7/2}$
29	$2\Gamma_6$	9115	8025	52.03 ${}^6H_{9/2}$ + 44.31 ${}^6F_{11/2}$ + 1.41 ${}^6F_{9/2}$
30	$\Gamma_{4,5}$		8049	61.74 ${}^6H_{9/2}$ + 35.05 ${}^6F_{11/2}$ + 1.76 ${}^6H_{7/2}$
31	$2\Gamma_6$		8100	52.62 ${}^6H_{9/2}$ + 44.60 ${}^6F_{11/2}$ + 0.86 ${}^6H_{11/2}$
32	$\Gamma_{4,5}$		8346	83.00 ${}^6F_{11/2}$ + 11.97 ${}^6H_{9/2}$ + 2.40 ${}^6H_{7/2}$
33	$\Gamma_{4,5}$		8991	68.08 ${}^6H_{7/2}$ + 30.28 ${}^6F_{9/2}$ + 0.54 ${}^6F_{11/2}$
34	$\Gamma_{4,5}$		9263	52.21 ${}^6F_{9/2}$ + 43.52 ${}^6H_{7/2}$ + 3.10 ${}^6H_{9/2}$
35	$\Gamma_{4,5}$		9274	61.34 ${}^6F_{9/2}$ + 34.78 ${}^6H_{7/2}$ + 1.49 ${}^6H_{9/2}$
36	$2\Gamma_6$		9287	81.55 ${}^6F_{9/2}$ + 14.90 ${}^6H_{7/2}$ + 2.42 ${}^6H_{5/2}$
37	$2\Gamma_6$		9359	66.03 ${}^6F_{9/2}$ + 30.28 ${}^6H_{7/2}$ + 1.59 ${}^6H_{5/2}$
38	$\Gamma_{4,5}$		9368	55.13 ${}^6H_{7/2}$ + 42.33 ${}^6F_{9/2}$ + 0.83 ${}^6H_{5/2}$
39	$\Gamma_{4,5}$		9456	66.60 ${}^6F_{9/2}$ + 30.07 ${}^6H_{7/2}$ + 1.06 ${}^6H_{9/2}$
40	$\Gamma_{4,5}$		9503	53.60 ${}^6H_{7/2}$ + 40.23 ${}^6F_{9/2}$ + 3.35 ${}^6H_{5/2}$
41	$2\Gamma_6$		9600	46.21 ${}^6F_{9/2}$ + 42.51 ${}^6H_{7/2}$ + 6.90 ${}^6H_{5/2}$
42	$\Gamma_{4,5}$	${}^6H_{5/2}$	10174	93.38 ${}^6H_{5/2}$ + 2.36 ${}^6F_{7/2}$ + 2.22 ${}^6F_{9/2}$
43	$2\Gamma_6$	10168	10423	85.46 ${}^6H_{5/2}$ + 9.64 ${}^6H_{7/2}$ + 2.05 ${}^6F_{7/2}$
44	$\Gamma_{4,5}$		10687	91.00 ${}^6H_{5/2}$ + 5.34 ${}^6F_{7/2}$ + 2.12 ${}^6H_{7/2}$
45	$\Gamma_{4,5}$	${}^6F_{7/2}$	11239	98.16 ${}^6F_{7/2}$ + 0.66 ${}^6H_{7/2}$ + 0.52 ${}^6H_{5/2}$
46	$2\Gamma_6$	11025	11281	96.24 ${}^6F_{7/2}$ + 1.97 ${}^6H_{5/2}$ + 0.84 ${}^6F_{5/2}$
47	$\Gamma_{4,5}$		11349	95.39 ${}^6F_{7/2}$ + 2.44 ${}^6H_{5/2}$ + 0.67 ${}^6H_{7/2}$
48	$\Gamma_{4,5}$		11407	93.45 ${}^6F_{7/2}$ + 3.65 ${}^6H_{5/2}$ + 1.01 ${}^6F_{5/2}$

Table 20. (cont'd)
Predicted energy
levels for Dy³⁺ in
Ca₅(PO₄)₃F, C₃ site.
B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm ⁻¹)	Free ion mixture (%)
49	Γ _{4,5}	⁶ F _{5/2}	12655	97.69 ⁶ F _{5/2} + 1.20 ⁶ F _{3/2} + 0.44 ⁶ H _{5/2}
50	Γ _{4,5}	12432	12705	97.29 ⁶ F _{5/2} + 0.70 ⁶ F _{3/2} + 0.69 ⁶ H _{7/2}
51	2Γ ₆		12767	96.67 ⁶ F _{5/2} + 1.62 ⁶ F _{3/2} + 0.52 ⁶ F _{7/2}
52	2Γ ₆	⁶ F _{3/2}	13489	97.28 ⁶ F _{3/2} + 1.34 ⁶ F _{5/2} + 0.85 ⁶ H _{5/2}
53	Γ _{4,5}	13212	13498	93.92 ⁶ F _{3/2} + 3.81 ⁶ F _{1/2} + 1.54 ⁶ F _{5/2}
54	Γ _{4,5}	⁶ F _{1/2} 13760	14060	95.11 ⁶ F _{1/2} + 3.33 ⁶ F _{3/2} + 0.50 ⁶ H _{5/2}
55	Γ _{4,5}	⁴ F _{9/2}	21143	97.63 ⁴ F _{9/2} + 1.81 ⁴ I _{15/2} + 0.55 ⁴ G _{11/2}
56	Γ _{4,5}	21144	21303	97.79 ⁴ F _{9/2} + 1.88 ⁴ I _{15/2} + 0.33 ⁴ G _{11/2}
57	2Γ ₆		21314	97.61 ⁴ F _{9/2} + 1.22 ⁴ G _{11/2} + 1.16 ⁴ I _{15/2}
58	Γ _{4,5}		21407	99.10 ⁴ F _{9/2} + 0.84 ⁴ I _{15/2} + 0.05 ⁴ G _{11/2}
59	2Γ ₆		21537	92.80 ⁴ F _{9/2} + 5.00 ⁴ I _{15/2} + 2.20 ⁴ G _{11/2}
60	Γ _{4,5}	⁴ I _{15/2}	22213	99.57 ⁴ I _{15/2} + 0.30 ⁴ G _{11/2} + 0.13 ⁴ F _{9/2}
61	Γ _{4,5}	22293	22282	98.82 ⁴ I _{15/2} + 1.06 ⁴ G _{11/2} + 0.12 ⁴ F _{9/2}
62	2Γ ₆		22413	94.96 ⁴ I _{15/2} + 4.90 ⁴ F _{9/2} + 0.14 ⁴ G _{11/2}
63	2Γ ₆		22576	99.36 ⁴ I _{15/2} + 0.48 ⁴ G _{11/2} + 0.16 ⁴ F _{9/2}
64	Γ _{4,5}		22609	94.40 ⁴ I _{15/2} + 3.40 ⁴ G _{11/2} + 2.20 ⁴ F _{9/2}
65	Γ _{4,5}		22696	95.48 ⁴ I _{15/2} + 3.59 ⁴ G _{11/2} + 0.93 ⁴ F _{9/2}
66	2Γ ₆		22710	94.88 ⁴ I _{15/2} + 4.14 ⁴ G _{11/2} + 0.97 ⁴ F _{9/2}
67	Γ _{4,5}		22730	96.66 ⁴ I _{15/2} + 2.12 ⁴ G _{11/2} + 1.22 ⁴ F _{9/2}
68	Γ _{4,5}	⁴ G _{11/2}	23278	97.69 ⁴ G _{11/2} + 2.24 ⁴ I _{15/2} + 0.07 ⁴ F _{9/2}
69	2Γ ₆	23321	23594	95.95 ⁴ G _{11/2} + 3.21 ⁴ F _{9/2} + 0.84 ⁴ I _{15/2}
70	Γ _{4,5}		23625	98.74 ⁴ G _{11/2} + 0.75 ⁴ I _{15/2} + 0.50 ⁴ F _{9/2}
71	Γ _{4,5}		23660	99.05 ⁴ G _{11/2} + 0.76 ⁴ I _{15/2} + 0.18 ⁴ F _{9/2}
72	2Γ ₆		23706	95.86 ⁴ G _{11/2} + 3.80 ⁴ I _{15/2} + 0.34 ⁴ F _{9/2}
73	Γ _{4,5}		23759	93.10 ⁴ G _{11/2} + 6.79 ⁴ I _{15/2} + 0.11 ⁴ F _{9/2}

^aIrreducible representations of C₃ double group, Γ_{4,5} = Γ₄ + Γ₅.

^bAqueous centroids (cm⁻¹).

Table 21. Predicted
energy levels for Ho³⁺
in Ca₅(PO₄)₃F, C₃ site.
B_{nm} from table 6.

Level	I. R. ^a	[(S,L)] ^b	Energy (cm ⁻¹)	Free ion mixture (%)
1	Γ _{2,3}	⁵ I ₈	0	99.89 ⁵ I ₈ + 0.09 ⁵ I ₇ + 0.01 ⁵ F ₅
2	Γ ₁	80	73	99.91 ⁵ I ₈ + 0.05 ⁵ I ₇ + 0.02 ⁵ I ₆
3	Γ ₁		86	99.91 ⁵ I ₈ + 0.05 ⁵ I ₇ + 0.03 ⁵ I ₆
4	Γ _{2,3}		157	99.93 ⁵ I ₈ + 0.05 ⁵ I ₇
5	Γ ₁		327	99.87 ⁵ I ₈ + 0.06 ⁵ I ₇ + 0.03 ⁵ G ₆
6	Γ _{2,3}		330	99.79 ⁵ I ₈ + 0.16 ⁵ I ₇ + 0.02 ⁵ G ₆
7	Γ _{2,3}		420	99.86 ⁵ I ₈ + 0.07 ⁵ I ₇ + 0.03 ⁵ G ₆
8	Γ ₁		444	99.90 ⁵ I ₈ + 0.04 ⁵ G ₆ + 0.02 ⁵ I ₇
9	Γ _{2,3}		460	99.81 ⁵ I ₈ + 0.16 ⁵ I ₇ + 0.01 ⁵ G ₆
10	Γ _{2,3}		480	99.88 ⁵ I ₈ + 0.07 ⁵ I ₇ + 0.02 ⁵ G ₆
11	Γ ₁		496	99.89 ⁵ I ₈ + 0.05 ⁵ I ₇ + 0.02 ⁵ G ₆
12	Γ ₁	⁵ I ₇	5200	99.74 ⁵ I ₇ + 0.16 ⁵ I ₆ + 0.08 ⁵ I ₈
13	Γ ₁	5116	5201	99.71 ⁵ I ₇ + 0.17 ⁵ I ₆ + 0.09 ⁵ I ₈
14	Γ _{2,3}		5238	99.53 ⁵ I ₇ + 0.24 ⁵ I ₈ + 0.14 ⁵ I ₆
15	Γ _{2,3}		5278	99.67 ⁵ I ₇ + 0.24 ⁵ I ₈ + 0.04 ⁵ I ₆
16	Γ _{2,3}		5324	99.55 ⁵ I ₇ + 0.36 ⁵ I ₆ + 0.04 ⁵ I ₈
17	Γ ₁		5362	99.56 ⁵ I ₇ + 0.30 ⁵ I ₆ + 0.06 ⁵ I ₅

Table 21 (cont'd).
Predicted energy
levels for Ho^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S, L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
18	Γ_1		5389	$99.75\ ^5I_7 + 0.15\ ^5I_6 + 0.04\ ^5I_8$
19	$\Gamma_{2,3}$		5435	$99.78\ ^5I_7 + 0.07\ ^5I_6 + 0.05\ ^5I_5$
20	$\Gamma_{2,3}$		5466	$99.84\ ^5I_7 + 0.04\ ^5I_8 + 0.03\ ^5F_5$
21	Γ_1		5475	$99.86\ ^5I_7 + 0.05\ ^5F_5 + 0.02\ ^5I_8$
22	Γ_1	5I_6	8757	$99.30\ ^5I_6 + 0.44\ ^5I_5 + 0.20\ ^5I_7$
23	$\Gamma_{2,3}$	8614	8758	$99.49\ ^5I_6 + 0.26\ ^5I_5 + 0.16\ ^5I_7$
24	Γ_1		8759	$99.45\ ^5I_6 + 0.32\ ^5I_5 + 0.16\ ^5I_7$
25	$\Gamma_{2,3}$		8761	$99.11\ ^5I_6 + 0.37\ ^5I_7 + 0.37\ ^5I_5$
26	Γ_1		8809	$99.48\ ^5I_6 + 0.25\ ^5I_7 + 0.12\ ^5I_5$
27	Γ_1		8818	$99.40\ ^5I_6 + 0.30\ ^5I_5 + 0.15\ ^5I_7$
28	$\Gamma_{2,3}$		8890	$99.51\ ^5I_6 + 0.29\ ^5I_5 + 0.06\ ^5F_5$
29	$\Gamma_{2,3}$		8972	$99.72\ ^5I_6 + 0.08\ ^5I_5 + 0.07\ ^5I_4$
30	Γ_1		9005	$99.85\ ^5I_6 + 0.04\ ^5I_4 + 0.03\ ^5F_4$
31	$\Gamma_{2,3}$	5I_5	11308	$98.88\ ^5I_5 + 0.63\ ^5I_4 + 0.38\ ^5I_6$
32	$\Gamma_{2,3}$	11164	11322	$99.30\ ^5I_5 + 0.37\ ^5I_6 + 0.22\ ^5I_4$
33	Γ_1		11329	$97.72\ ^5I_5 + 1.72\ ^5I_4 + 0.38\ ^5I_6$
34	Γ_1		11345	$98.35\ ^5I_5 + 0.79\ ^5I_6 + 0.75\ ^5I_4$
35	$\Gamma_{2,3}$		11425	$99.54\ ^5I_5 + 0.18\ ^5I_4 + 0.17\ ^5I_6$
36	$\Gamma_{2,3}$		11490	$99.18\ ^5I_5 + 0.61\ ^5I_4 + 0.07\ ^5I_6$
37	Γ_1		11535	$99.78\ ^5I_5 + 0.08\ ^5F_5 + 0.03\ ^5F_1$
38	Γ_1	5I_4	13218	$99.23\ ^5I_4 + 0.58\ ^5I_5 + 0.11\ ^5I_6$
39	Γ_1	13219	13329	$98.14\ ^5I_4 + 1.75\ ^5I_5 + 0.06\ ^5I_6$
40	$\Gamma_{2,3}$		13363	$99.14\ ^5I_4 + 0.64\ ^5I_5 + 0.13\ ^5I_6$
41	$\Gamma_{2,3}$		13520	$98.98\ ^5I_4 + 0.82\ ^5I_5 + 0.05\ ^5I_6$
42	Γ_1		13568	$99.59\ ^5I_4 + 0.15\ ^5I_5 + 0.11\ ^5S_2$
43	$\Gamma_{2,3}$		13635	$99.65\ ^5I_4 + 0.18\ ^5I_5 + 0.05\ ^5F_3$
44	Γ_1	5F_5	15602	$99.38\ ^5F_5 + 0.34\ ^5G_6 + 0.13\ ^5F_4$
45	Γ_1	15519	15620	$99.31\ ^5F_5 + 0.35\ ^5G_6 + 0.18\ ^5F_4$
46	$\Gamma_{2,3}$		15653	$99.32\ ^5F_5 + 0.29\ ^5F_4 + 0.23\ ^5G_6$
47	$\Gamma_{2,3}$		15670	$99.39\ ^5F_5 + 0.25\ ^5G_6 + 0.15\ ^5F_4$
48	$\Gamma_{2,3}$		15771	$99.52\ ^5F_5 + 0.15\ ^5F_4 + 0.11\ ^5G_6$
49	Γ_1		15800	$99.68\ ^5F_5 + 0.08\ ^5I_5 + 0.07\ ^5F_4$
50	$\Gamma_{2,3}$		15950	$99.87\ ^5F_5 + 0.05\ ^3G_5 + 0.03\ ^5G_6$
51	Γ_1	5S_2	18558	$93.92\ ^5S_2 + 5.72\ ^5F_4 + 0.17\ ^5G_6$
52	$\Gamma_{2,3}$	18353	18571	$95.68\ ^5S_2 + 3.99\ ^5F_4 + 0.20\ ^5G_6$
53	$\Gamma_{2,3}$		18588	$97.36\ ^5S_2 + 2.27\ ^5F_4 + 0.18\ ^5G_6$
54	Γ_1	5F_4	18682	$93.62\ ^5F_4 + 5.37\ ^5S_2 + 0.56\ ^5G_6$
55	$\Gamma_{2,3}$	18612	18747	$95.14\ ^5F_4 + 3.97\ ^5S_2 + 0.49\ ^5G_6$
56	Γ_1		18849	$98.84\ ^5F_4 + 0.54\ ^5F_3 + 0.18\ ^5G_6$
57	$\Gamma_{2,3}$		18857	$97.07\ ^5F_4 + 2.13\ ^5S_2 + 0.24\ ^5F_2$
58	Γ_1		18884	$98.46\ ^5F_4 + 0.91\ ^5F_3 + 0.17\ ^5F_5$
59	$\Gamma_{2,3}$		18968	$98.93\ ^5F_4 + 0.53\ ^5F_5 + 0.18\ ^5S_2$
60	Γ_1	5F_3	20759	$98.84\ ^5F_3 + 0.62\ ^3G_5 + 0.24\ ^5F_4$
61	$\Gamma_{2,3}$	20672	20805	$97.81\ ^5F_3 + 1.15\ ^5F_2 + 0.47\ ^3G_5$
62	Γ_1		20949	$98.02\ ^5F_3 + 0.95\ ^5G_6 + 0.72\ ^5F_4$
63	$\Gamma_{2,3}$		20976	$93.11\ ^5F_3 + 6.06\ ^5F_2 + 0.37\ ^5G_6$
64	Γ_1		20990	$98.08\ ^5F_3 + 0.85\ ^5F_4 + 0.77\ ^5G_6$

Table 21 (cont'd).
Predicted energy
levels for Ho^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
65	Γ_1	5F_2	21252	$98.50 ^5F_2 + 0.98 ^5G_6 + 0.31 ^3K_8$
66	$\Gamma_{2,3}$	21130	21371	$94.83 ^5F_2 + 2.36 ^5F_3 + 1.22 ^3K_8$
67	$\Gamma_{2,3}$		21430	$90.77 ^5F_2 + 4.35 ^5F_3 + 3.23 ^3K_8$
68	Γ_1	3K_8	21467	$99.31 ^3K_8 + 0.49 ^5G_6 + 0.18 ^5F_2$
69	$\Gamma_{2,3}$	21307	21471	$98.34 ^3K_8 + 1.04 ^5F_2 + 0.50 ^5G_6$
70	$\Gamma_{2,3}$		21481	$98.26 ^3K_8 + 1.47 ^5F_2 + 0.22 ^5F_3$
71	Γ_1		21483	$99.48 ^3K_8 + 0.36 ^5G_6 + 0.11 ^5F_2$
72	$\Gamma_{2,3}$		21491	$98.32 ^3K_8 + 1.25 ^5F_2 + 0.35 ^5G_6$
73	Γ_1		21518	$98.54 ^3K_8 + 1.39 ^5G_6 + 0.03 ^5F_2$
74	$\Gamma_{2,3}$		21524	$99.32 ^3K_8 + 0.32 ^5G_6 + 0.26 ^5F_2$
75	$\Gamma_{2,3}$		21597	$99.64 ^3K_8 + 0.18 ^5G_6 + 0.15 ^5F_2$
76	Γ_1		21616	$98.18 ^3K_8 + 1.69 ^5G_6 + 0.11 ^5F_3$
77	Γ_1		21622	$98.65 ^3K_8 + 1.27 ^5G_6 + 0.07 ^5F_3$
78	$\Gamma_{2,3}$		21654	$99.88 ^3K_8 + 0.10 ^5G_6 + 0.01 ^5F_2$
79	Γ_1	5G_6	22181	$97.77 ^5G_6 + 0.67 ^5F_2 + 0.63 ^3K_8$
80	Γ_1	22094	22191	$96.85 ^5G_6 + 1.90 ^3K_8 + 0.89 ^5F_1$
81	Γ_1	5F_1	22209	$96.93 ^5G_6 + 2.04 ^3K_8 + 0.37 ^5F_3$
82	$\Gamma_{2,3}$	22375	22229	$97.30 ^5G_6 + 0.58 ^5F_2 + 0.58 ^3G_5$
83	$\Gamma_{2,3}$		22320	$97.43 ^5G_6 + 0.89 ^3G_5 + 0.62 ^5F_1$
84	$\Gamma_{2,3}$		22420	$97.05 ^5G_6 + 1.19 ^5F_1 + 0.85 ^3G_5$
85	Γ_1		22467	$66.37 ^5G_6 + 32.81 ^5F_1 + 0.28 ^3K_8$
86	Γ_1		22513	$73.74 ^5G_6 + 25.05 ^5F_1 + 0.35 ^3K_8$
87	$\Gamma_{2,3}$		22516	$94.51 ^5G_6 + 3.16 ^5F_1 + 0.98 ^3G_5$
88	Γ_1		22554	$58.01 ^5G_6 + 40.80 ^5F_1 + 0.60 ^5F_3$
89	$\Gamma_{2,3}$		22703	$93.02 ^5F_1 + 5.42 ^5G_6 + 0.73 ^5F_2$
90	Γ_1	3G_5	24043	$99.23 ^3G_5 + 0.67 ^5F_3 + 0.04 ^5F_5$
91	$\Gamma_{2,3}$	23887	24065	$98.77 ^3G_5 + 0.41 ^5G_6 + 0.34 ^5F_3$
92	$\Gamma_{2,3}$		24096	$98.84 ^3G_5 + 0.63 ^5G_6 + 0.20 ^5F_2$
93	Γ_1		24158	$99.73 ^3G_5 + 0.12 ^5G_6 + 0.10 ^5F_4$
94	Γ_1		24175	$99.62 ^3G_5 + 0.19 ^5G_6 + 0.05 ^5F_4$
95	$\Gamma_{2,3}$		24219	$98.50 ^3G_5 + 1.19 ^5G_6 + 0.11 ^5F_2$
96	$\Gamma_{2,3}$		24265	$98.76 ^3G_5 + 0.98 ^5G_6 + 0.10 ^5F_4$

^aIrreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.

^bAqueous centroids (cm^{-1}).

Table 22. Predicted
energy levels for
 Tm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$,
 C_3 site. B_{nm} from table
6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	3H_6	0	$99.76 ^3H_6 + 0.20 ^3F_4 + 0.02 ^3H_4$
2	$\Gamma_{2,3}$	202	56	$99.82 ^3H_6 + 0.12 ^3F_4 + 0.03 ^3F_3$
3	$\Gamma_{2,3}$		186	$99.79 ^3H_6 + 0.14 ^3F_4 + 0.03 ^3H_5$
4	Γ_1		329	$99.56 ^3H_6 + 0.35 ^3F_4 + 0.06 ^3H_5$
5	Γ_1		418	$99.60 ^3H_6 + 0.28 ^3F_4 + 0.09 ^3H_5$
6	$\Gamma_{2,3}$		657	$99.60 ^3H_6 + 0.32 ^3F_4 + 0.06 ^3H_5$
7	Γ_1		659	$99.90 ^3H_6 + 0.08 ^3F_4 + 0.01 ^3H_4$
8	Γ_1		661	$99.88 ^3H_6 + 0.10 ^3F_4 + 0.01 ^3H_4$
9	$\Gamma_{2,3}$		896	$99.95 ^3H_6 + 0.03 ^3H_5 + 0.01 ^3F_3$

Table 22 (cont'd).
Predicted energy
levels for Tm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
10	$\Gamma_{2,3}$	3F_4	5834	$99.46\ ^3F_4 + 0.25\ ^3H_6 + 0.21\ ^3H_5$
11	Γ_1	5812	5843	$99.66\ ^3F_4 + 0.13\ ^3H_4 + 0.11\ ^3H_5$
12	$\Gamma_{2,3}$		6068	$99.03\ ^3F_4 + 0.71\ ^3H_5 + 0.17\ ^3H_6$
13	Γ_1		6171	$99.10\ ^3F_4 + 0.57\ ^3H_6 + 0.31\ ^3H_5$
14	Γ_1		6211	$98.50\ ^3F_4 + 1.00\ ^3H_5 + 0.47\ ^3H_6$
15	$\Gamma_{2,3}$		6226	$99.35\ ^3F_4 + 0.38\ ^3H_5 + 0.17\ ^3H_6$
16	Γ_1	3H_5	8263	$99.72\ ^3H_5 + 0.18\ ^3F_4 + 0.07\ ^3F_3$
17	$\Gamma_{2,3}$	8390	8312	$98.90\ ^3H_5 + 0.72\ ^3F_4 + 0.14\ ^3F_2$
18	$\Gamma_{2,3}$		8460	$99.38\ ^3H_5 + 0.23\ ^3F_3 + 0.20\ ^3H_4$
19	Γ_1		8697	$99.17\ ^3H_5 + 0.35\ ^3F_3 + 0.33\ ^3F_4$
20	Γ_1		8748	$98.55\ ^3H_5 + 0.93\ ^3F_4 + 0.37\ ^3F_3$
21	$\Gamma_{2,3}$		8893	$99.68\ ^3H_5 + 0.22\ ^3F_4 + 0.03\ ^3F_2$
22	$\Gamma_{2,3}$		8969	$99.49\ ^3H_5 + 0.27\ ^3F_4 + 0.17\ ^3H_4$
23	$\Gamma_{2,3}$	3H_4	12715	$98.26\ ^3H_4 + 0.97\ ^3F_2 + 0.52\ ^3F_3$
24	Γ_1	12720	12744	$98.44\ ^3H_4 + 1.34\ ^3F_3 + 0.12\ ^3F_4$
25	$\Gamma_{2,3}$		12875	$98.66\ ^3H_4 + 0.95\ ^3F_2 + 0.20\ ^3H_5$
26	$\Gamma_{2,3}$		13102	$99.11\ ^3H_4 + 0.46\ ^3F_3 + 0.18\ ^3H_5$
27	Γ_1		13160	$97.74\ ^3H_4 + 2.02\ ^3F_3 + 0.12\ ^3H_5$
28	Γ_1		13240	$97.15\ ^3H_4 + 2.63\ ^3F_3 + 0.08\ ^3H_5$
29	Γ_1	3F_3	14675	$97.39\ ^3F_3 + 2.19\ ^3H_4 + 0.31\ ^3H_5$
30	Γ_1		14742	$95.56\ ^3F_3 + 3.80\ ^3H_4 + 0.30\ ^3F_2$
31	$\Gamma_{2,3}$		14763	$96.88\ ^3F_3 + 2.65\ ^3F_2 + 0.26\ ^3H_5$
32	Γ_1		14801	$99.79\ ^3F_3 + 0.10\ ^3H_5 + 0.07\ ^3H_4$
33	$\Gamma_{2,3}$		14845	$94.36\ ^3F_3 + 4.84\ ^3F_2 + 0.61\ ^3H_4$
34	$\Gamma_{2,3}$	3F_2	15277	$95.30\ ^3F_2 + 3.11\ ^3F_3 + 1.38\ ^3H_4$
35	$\Gamma_{2,3}$	15116	15445	$94.71\ ^3F_2 + 4.03\ ^3F_3 + 1.02\ ^3H_4$
36	Γ_1		15597	$99.33\ ^3F_2 + 0.34\ ^3F_3 + 0.12\ ^3H_4$
37	Γ_1	1G_4	21188	$99.86\ ^1G_4 + 0.05\ ^3P_2 + 0.03\ ^3F_3$
38	$\Gamma_{2,3}$	21374	21322	$99.78\ ^1G_4 + 0.05\ ^3F_3 + 0.05\ ^1I_6$
39	$\Gamma_{2,3}$		21697	$99.84\ ^1G_4 + 0.09\ ^1I_6 + 0.03\ ^3H_4$
40	$\Gamma_{2,3}$		21802	$99.72\ ^1G_4 + 0.17\ ^1D_2 + 0.03\ ^1I_6$
41	Γ_1		21816	$99.88\ ^1G_4 + 0.04\ ^3F_3 + 0.04\ ^1I_6$
42	Γ_1		21904	$99.90\ ^1G_4 + 0.05\ ^1I_6 + 0.03\ ^3H_5$
43	$\Gamma_{2,3}$	1D_2	28098	$99.69\ ^1D_2 + 0.17\ ^1G_4 + 0.10\ ^1I_6$
44	$\Gamma_{2,3}$	28032	28387	$99.60\ ^1D_2 + 0.21\ ^3P_1 + 0.06\ ^1I_6$
45	Γ_1		28451	$99.77\ ^1D_2 + 0.07\ ^3F_2 + 0.04\ ^3P_0$
46	Γ_1	1I_6	34674	$99.96\ ^1I_6 + 0.02\ ^1G_4 + 0.02\ ^3P_2$
47	$\Gamma_{2,3}$	34886	34716	$99.63\ ^1I_6 + 0.26\ ^3P_2 + 0.07\ ^1D_2$
48	$\Gamma_{2,3}$	3P_0	34793	$99.68\ ^1I_6 + 0.22\ ^3P_2 + 0.06\ ^1D_2$
49	Γ_1	35637	34824	$99.95\ ^1I_6 + 0.04\ ^1G_4 + 0.01\ ^3P_0$
50	Γ_1	3P_1	34946	$99.71\ ^1I_6 + 0.21\ ^3P_0 + 0.03\ ^1G_4$
51	$\Gamma_{2,3}$	36297	35030	$99.79\ ^1I_6 + 0.10\ ^1G_4 + 0.06\ ^3P_2$
52	$\Gamma_{2,3}$		35356	$99.91\ ^1I_6 + 0.06\ ^3P_2 + 0.01\ ^1D_2$
53	Γ_1		35880	$98.18\ ^3P_0 + 0.90\ ^3P_2 + 0.81\ ^1I_6$
54	Γ_1		36289	$58.43\ ^3P_1 + 41.56\ ^1I_6 + 0.01\ ^3F_3$
55	Γ_1		36295	$99.17\ ^1I_6 + 0.64\ ^3P_0 + 0.08\ ^3P_1$
56	Γ_1		36298	$58.51\ ^1I_6 + 41.48\ ^3P_1$
57	$\Gamma_{2,3}$		36677	$97.84\ ^3P_1 + 1.87\ ^3P_2 + 0.20\ ^1D_2$

Table 22 (cont'd).
Predicted energy
levels for Tm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
58	$\Gamma_{2,3}$	3P_2	38196	$99.47\ ^3P_2 + 0.37\ ^1I_6 + 0.12\ ^3P_1$
59	$\Gamma_{2,3}$	38193	38525	$97.96\ ^3P_2 + 1.74\ ^3P_1 + 0.22\ ^1I_6$
60	Γ_1		38960	$98.89\ ^3P_2 + 0.84\ ^3P_0 + 0.17\ ^1I_6$
61	Γ_1	1S_0 79592	79855	$99.97\ ^1S_0 + 0.01\ ^3P_2 + 0.01\ ^1G_4$

^aIrreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.

^bAqueous centroid (cm^{-1}).

Table 23. Predicted
energy levels for Yb^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_3 site.
 B_{nm} from table 6.

Level	I. R. ^a	$[(S,L)]^b$	Energy (cm^{-1})	Free ion mixture (%)
1	$2\Gamma_6$	$^2F_{7/2}$	0	$99.97\ ^2F_{7/2} + 0.03\ ^2F_{5/2}$
2	$\Gamma_{4,5}$	250	52	$99.92\ ^2F_{7/2} + 0.08\ ^2F_{5/2}$
3	$\Gamma_{4,5}$		318	$99.96\ ^2F_{7/2} + 0.04\ ^2F_{5/2}$
4	$\Gamma_{4,5}$		891	$99.98\ ^2F_{7/2} + 0.02\ ^2F_{5/2}$
5	$2\Gamma_6$	$^2F_{5/2}$	10231	$99.97\ ^2F_{5/2} + 0.03\ ^2F_{7/2}$
6	$\Gamma_{4,5}$	10450	10359	$99.94\ ^2F_{5/2} + 0.06\ ^2F_{7/2}$
7	$\Gamma_{4,5}$		10988	$99.92\ ^2F_{5/2} + 0.08\ ^2F_{7/2}$

^aIrreducible representations of C_3 double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.

^bAqueous centroids (cm^{-1}).

Table 24. Predicted
energy levels for Ce^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	$^2F_{5/2}$	0	$98.03\ ^2F_{5/2} + 1.97\ ^2F_{7/2}$
2	250	561	$93.72\ ^2F_{5/2} + 6.28\ ^2F_{7/2}$
3		1263	$90.08\ ^2F_{5/2} + 9.92\ ^2F_{7/2}$
4	$^2F_{7/2}$	2330	$93.56\ ^2F_{7/2} + 6.44\ ^2F_{5/2}$
5	2550	2819	$92.32\ ^2F_{7/2} + 7.68\ ^2F_{5/2}$
6		3455	$98.45\ ^2F_{7/2} + 1.55\ ^2F_{5/2}$
7		3859	$97.50\ ^2F_{7/2} + 2.50\ ^2F_{5/2}$

^aAqueous centroids (cm^{-1}).

Table 25. Predicted
energy levels for Pr^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	3H_4	0	$98.23\ ^3H_4 + 1.09\ ^3H_5 + 0.29\ ^3F_2$
2	Γ_1	245	61	$97.36\ ^3H_4 + 2.10\ ^3H_5 + 0.23\ ^3F_3$
3	Γ_2		509	$95.53\ ^3H_4 + 3.07\ ^3H_5 + 1.07\ ^3F_2$
4	Γ_1		636	$97.19\ ^3H_4 + 1.51\ ^3H_5 + 0.82\ ^3F_2$
5	Γ_2		655	$97.81\ ^3H_4 + 1.58\ ^3H_5 + 0.41\ ^3F_2$
6	Γ_2		766	$97.00\ ^3H_4 + 2.32\ ^3H_5 + 0.50\ ^3F_2$
7	Γ_1		1072	$97.42\ ^3H_4 + 1.29\ ^3F_2 + 0.93\ ^3H_5$
8	Γ_1		1151	$98.36\ ^3H_4 + 0.58\ ^3F_3 + 0.53\ ^3H_5$
9	Γ_2		1240	$97.59\ ^3H_4 + 1.50\ ^3H_5 + 0.77\ ^3F_3$

Table 25 (cont'd).
Predicted energy
levels for Pr^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
10	Γ_2	3H_5	2164	$95.69\ ^3H_5 + 2.09\ ^3H_4 + 1.03\ ^3H_6$
11	Γ_2	2323	2205	$94.50\ ^3H_5 + 3.27\ ^3H_4 + 1.51\ ^3H_6$
12	Γ_1		2587	$94.67\ ^3H_5 + 2.26\ ^3H_4 + 1.12\ ^3F_3$
13	Γ_2		2643	$95.94\ ^3H_5 + 1.78\ ^3H_6 + 1.37\ ^3F_3$
14	Γ_1		2654	$94.93\ ^3H_5 + 2.65\ ^3H_6 + 1.33\ ^3H_4$
15	Γ_1		2702	$94.74\ ^3H_5 + 2.91\ ^3H_6 + 1.06\ ^3F_2$
16	Γ_2		2970	$95.42\ ^3H_5 + 1.55\ ^3F_2 + 1.28\ ^3H_4$
17	Γ_2		3051	$97.46\ ^3H_5 + 0.90\ ^3F_3 + 0.72\ ^3H_4$
18	Γ_1		3085	$94.18\ ^3H_5 + 1.50\ ^3H_4 + 1.49\ ^3H_6$
19	Γ_1		3196	$95.79\ ^3H_5 + 1.38\ ^3H_6 + 1.05\ ^3F_2$
20	Γ_2		3200	$96.33\ ^3H_5 + 1.27\ ^3F_2 + 0.92\ ^3F_4$
21	Γ_1	3H_6	4214	$95.37\ ^3H_6 + 2.23\ ^3H_5 + 1.13\ ^3F_4$
22	Γ_1	4496	4226	$94.14\ ^3H_6 + 3.41\ ^3H_5 + 1.27\ ^3F_4$
23	Γ_2		4558	$94.47\ ^3H_6 + 2.28\ ^3H_5 + 1.77\ ^3F_4$
24	Γ_1		4669	$93.45\ ^3H_6 + 3.38\ ^3F_4 + 1.25\ ^3H_5$
25	Γ_2		4748	$95.19\ ^3H_6 + 1.79\ ^3H_5 + 1.26\ ^3F_2$
26	Γ_2		4875	$96.45\ ^3H_6 + 1.50\ ^3F_4 + 0.89\ ^3F_3$
27	Γ_1		5066	$92.29\ ^3H_6 + 3.95\ ^3F_2 + 1.77\ ^3F_3$
28	Γ_1		5116	$92.89\ ^3H_6 + 3.52\ ^3F_3 + 1.99\ ^3F_4$
29	Γ_2		5192	$82.42\ ^3H_6 + 15.26\ ^3F_2 + 0.97\ ^3F_4$
30	Γ_2		5280	$88.59\ ^3H_6 + 3.86\ ^3F_2 + 3.73\ ^3F_4$
31	Γ_1		5327	$84.53\ ^3H_6 + 10.92\ ^3F_2 + 1.82\ ^3F_4$
32	Γ_1		5351	$87.51\ ^3H_6 + 4.50\ ^3F_2 + 4.15\ ^3F_4$
33	Γ_2		5374	$92.93\ ^3H_6 + 3.14\ ^3F_3 + 2.72\ ^3F_4$
34	Γ_1	3F_2	5648	$80.91\ ^3F_2 + 15.29\ ^3H_6 + 2.11\ ^3H_5$
35	Γ_2	5149	5738	$81.02\ ^3F_2 + 15.94\ ^3H_6 + 1.22\ ^3H_5$
36	Γ_2		5774	$89.46\ ^3F_2 + 4.86\ ^3H_6 + 2.91\ ^3H_5$
37	Γ_1		5873	$93.89\ ^3F_2 + 2.37\ ^3H_6 + 1.64\ ^3H_5$
38	Γ_1		5907	$91.77\ ^3F_2 + 4.80\ ^3H_6 + 1.59\ ^3H_5$
39	Γ_2	3F_3	7012	$93.14\ ^3F_3 + 5.32\ ^3F_4 + 0.76\ ^3H_6$
40	Γ_1	6540	7014	$82.56\ ^3F_3 + 11.98\ ^3F_4 + 3.68\ ^3H_6$
41	Γ_1		7070	$80.00\ ^3F_3 + 13.53\ ^3F_4 + 4.69\ ^3H_6$
42	Γ_2		7128	$87.40\ ^3F_3 + 5.92\ ^3F_4 + 3.69\ ^3H_6$
43	Γ_1		7160	$58.99\ ^3F_3 + 34.45\ ^3F_4 + 3.06\ ^3H_6$
44	Γ_2		7177	$67.64\ ^3F_3 + 27.02\ ^3F_4 + 3.56\ ^3H_6$
45	Γ_2		7267	$83.86\ ^3F_3 + 11.55\ ^3F_4 + 2.77\ ^3H_6$
46	Γ_1	3F_4	7297	$88.69\ ^3F_4 + 7.68\ ^3F_3 + 1.41\ ^1G_4$
47	Γ_1	6973	7390	$64.44\ ^3F_4 + 32.78\ ^3F_3 + 1.53\ ^1G_4$
48	Γ_2		7403	$62.76\ ^3F_4 + 32.72\ ^3F_3 + 2.77\ ^3H_6$
49	Γ_1		7509	$74.57\ ^3F_4 + 15.91\ ^3F_3 + 8.01\ ^3H_6$
50	Γ_2		7538	$83.05\ ^3F_4 + 12.97\ ^3F_3 + 3.11\ ^3H_6$
51	Γ_2		7643	$97.09\ ^3F_4 + 1.20\ ^3H_6 + 0.80\ ^3H_5$
52	Γ_1		7771	$94.26\ ^3F_4 + 2.94\ ^3F_3 + 1.38\ ^3H_6$
53	Γ_2		7865	$90.96\ ^3F_4 + 4.96\ ^3F_3 + 3.25\ ^3H_6$
54	Γ_1		7870	$94.45\ ^3F_4 + 2.57\ ^3H_6 + 1.90\ ^3F_3$
55	Γ_2	1G_4	9967	$97.40\ ^1G_4 + 1.07\ ^3F_4 + 0.90\ ^3H_6$
56	Γ_1	9885	9982	$96.96\ ^1G_4 + 2.08\ ^3F_4 + 0.35\ ^3H_6$
57	Γ_1		10015	$97.92\ ^1G_4 + 1.24\ ^3F_4 + 0.40\ ^3H_6$
58	Γ_1		10135	$98.08\ ^1G_4 + 0.91\ ^3H_6 + 0.40\ ^3F_4$

Table 25 (cont'd).
Predicted energy
levels for Pr^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
59	Γ_2		10417	$99.42\ ^1G_4 + 0.14\ ^3H_6 + 0.11\ ^3F_4$
60	Γ_2		10535	$99.27\ ^1G_4 + 0.26\ ^1I_6 + 0.13\ ^3H_6$
61	Γ_1		10722	$99.23\ ^1G_4 + 0.23\ ^1I_6 + 0.19\ ^3H_6$
62	Γ_2		10873	$98.81\ ^1G_4 + 0.49\ ^3F_4 + 0.24\ ^3H_6$
63	Γ_1		11010	$98.49\ ^1G_4 + 0.94\ ^3F_4 + 0.27\ ^1I_6$
64	Γ_2	1D_2	16651	$98.71\ ^1D_2 + 0.67\ ^1I_6 + 0.18\ ^3P_2$
65	Γ_1	16840	17156	$99.04\ ^1D_2 + 0.41\ ^1I_6 + 0.24\ ^1G_4$
66	Γ_1		17467	$98.99\ ^1D_2 + 0.84\ ^1I_6 + 0.05\ ^1G_4$
67	Γ_2		17494	$98.47\ ^1D_2 + 0.95\ ^1I_6 + 0.20\ ^3P_1$
68	Γ_1		17943	$98.72\ ^1D_2 + 0.91\ ^1I_6 + 0.13\ ^3P_2$
69	Γ_1	3P_0	20934	$99.19\ ^1I_6 + 0.44\ ^1D_2 + 0.15\ ^1G_4$
70	Γ_1	20706	20944	$99.06\ ^1I_6 + 0.45\ ^1D_2 + 0.17\ ^1G_4$
71	Γ_2	3P_1	21178	$99.33\ ^1I_6 + 0.23\ ^1D_2 + 0.16\ ^1G_4$
72	Γ_1	21330	21194	$94.00\ ^3P_0 + 5.19\ ^3P_2 + 0.33\ ^1I_6$
73	Γ_2	1I_6	21199	$99.25\ ^1I_6 + 0.29\ ^1D_2 + 0.15\ ^3P_1$
74	Γ_2	21500	21613	$90.85\ ^3P_1 + 8.35\ ^3P_2 + 0.35\ ^1I_6$
75	Γ_2	3P_2	21662	$88.68\ ^3P_1 + 9.64\ ^3P_2 + 1.21\ ^1I_6$
76	Γ_1	22535	21951	$99.68\ ^1I_6 + 0.11\ ^1G_4 + 0.06\ ^3P_2$
77	Γ_1		22007	$98.80\ ^1I_6 + 0.47\ ^3P_2 + 0.29\ ^1D_2$
78	Γ_1		22190	$98.89\ ^3P_1 + 0.37\ ^3P_2 + 0.36\ ^1I_6$
79	Γ_2		22232	$99.26\ ^1I_6 + 0.37\ ^3P_1 + 0.14\ ^1D_2$
80	Γ_2		22341	$96.22\ ^1I_6 + 1.55\ ^3P_1 + 1.39\ ^3P_2$
81	Γ_1		22450	$98.11\ ^1I_6 + 1.02\ ^3P_2 + 0.36\ ^1D_2$
82	Γ_2		22634	$92.41\ ^1I_6 + 5.86\ ^3P_2 + 1.26\ ^3P_1$
83	Γ_1		22638	$89.75\ ^1I_6 + 9.10\ ^3P_2 + 0.75\ ^3P_0$
84	Γ_1		22959	$85.44\ ^3P_2 + 9.72\ ^1I_6 + 4.37\ ^3P_0$
85	Γ_2		22978	$78.21\ ^3P_2 + 14.25\ ^1I_6 + 6.94\ ^3P_1$
86	Γ_1		23071	$93.59\ ^1I_6 + 5.77\ ^3P_2 + 0.26\ ^1G_4$
87	Γ_2		23076	$85.26\ ^1I_6 + 13.15\ ^3P_2 + 1.16\ ^3P_1$
88	Γ_2		23216	$82.15\ ^3P_2 + 9.76\ ^1I_6 + 7.90\ ^3P_1$
89	Γ_1		23409	$93.26\ ^3P_2 + 6.22\ ^1I_6 + 0.15\ ^3P_0$
90	Γ_1		23457	$97.98\ ^3P_2 + 1.34\ ^1I_6 + 0.26\ ^3P_1$
91	Γ_1	1S_0	47471	$99.85\ ^1S_0 + 0.05\ ^1G_4 + 0.05\ ^1D_2$
		469001		

^aAqueous centroids (cm^{-1}).

Table 26. Predicted
energy levels for Nd^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	$^4I_{9/2}$	0	$98.91\ ^4I_{9/2} + 0.94\ ^4I_{11/2} + 0.05\ ^4I_{13/2}$
2	130	205	$98.67\ ^4I_{9/2} + 1.09\ ^4I_{11/2} + 0.10\ ^4I_{13/2}$
3		320	$98.13\ ^4I_{9/2} + 1.68\ ^4I_{11/2} + 0.07\ ^4I_{13/2}$
4		451	$98.99\ ^4I_{9/2} + 0.76\ ^4I_{11/2} + 0.10\ ^4I_{13/2}$
5		647	$98.64\ ^4I_{9/2} + 1.12\ ^4I_{11/2} + 0.09\ ^4I_{13/2}$
6	$^4I_{11/2}$	1977	$98.15\ ^4I_{11/2} + 0.94\ ^4I_{9/2} + 0.77\ ^4I_{13/2}$
7	2006	2121	$97.61\ ^4I_{11/2} + 1.56\ ^4I_{13/2} + 0.64\ ^4I_{9/2}$
8		2153	$98.08\ ^4I_{11/2} + 0.96\ ^4I_{9/2} + 0.84\ ^4I_{13/2}$
9		2311	$98.12\ ^4I_{11/2} + 0.89\ ^4I_{13/2} + 0.75\ ^4I_{9/2}$
10		2346	$97.72\ ^4I_{11/2} + 1.30\ ^4I_{9/2} + 0.79\ ^4I_{13/2}$
11		2443	$97.91\ ^4I_{11/2} + 1.03\ ^4I_{9/2} + 0.87\ ^4I_{13/2}$

Table 26 (cont'd).
Predicted energy
levels for Nd³⁺ in
Ca₅(PO₄)₃F, C_s site.
B_{nm} from table 9.

Level	[(S,L)] ^a	Energy (cm ⁻¹)	Free ion mixture (%)
12	⁴ I _{13/2}	3946	98.36 ⁴ I _{13/2} + 0.96 ⁴ I _{11/2} + 0.52 ⁴ I _{15/2}
13	4004	4075	97.75 ⁴ I _{13/2} + 1.16 ⁴ I _{15/2} + 0.88 ⁴ I _{11/2}
14		4119	98.57 ⁴ I _{13/2} + 0.86 ⁴ I _{15/2} + 0.41 ⁴ I _{11/2}
15		4270	97.70 ⁴ I _{13/2} + 1.06 ⁴ I _{15/2} + 1.03 ⁴ I _{11/2}
16		4325	98.55 ⁴ I _{13/2} + 0.86 ⁴ I _{15/2} + 0.45 ⁴ I _{11/2}
17		4394	97.74 ⁴ I _{13/2} + 1.34 ⁴ I _{11/2} + 0.79 ⁴ I _{15/2}
18		4491	98.53 ⁴ I _{13/2} + 0.72 ⁴ I _{11/2} + 0.54 ⁴ I _{15/2}
19	⁴ I _{15/2}	5913	98.82 ⁴ I _{15/2} + 1.01 ⁴ I _{13/2} + 0.06 ⁴ I _{11/2}
20	6080	6026	98.66 ⁴ I _{15/2} + 1.03 ⁴ I _{13/2} + 0.13 ⁴ F _{9/2}
21		6112	99.11 ⁴ I _{15/2} + 0.64 ⁴ I _{13/2} + 0.08 ⁴ F _{9/2}
22		6315	99.19 ⁴ I _{15/2} + 0.56 ⁴ I _{13/2} + 0.08 ⁴ F _{9/2}
23		6381	99.31 ⁴ I _{15/2} + 0.47 ⁴ I _{13/2} + 0.07 ⁴ F _{9/2}
24		6515	99.27 ⁴ I _{15/2} + 0.60 ⁴ I _{13/2} + 0.05 ⁴ I _{11/2}
25		6576	98.88 ⁴ I _{15/2} + 0.97 ⁴ I _{13/2} + 0.03 ⁴ F _{9/2}
26		6722	99.24 ⁴ I _{15/2} + 0.53 ⁴ I _{13/2} + 0.05 ⁴ F _{9/2}
27	⁴ F _{3/2}	11604	96.26 ⁴ F _{3/2} + 2.55 ⁴ F _{5/2} + 0.48 ⁴ F _{7/2}
28	11526	11793	94.10 ⁴ F _{3/2} + 3.23 ⁴ F _{5/2} + 1.07 ⁴ F _{7/2}
29	⁴ F _{5/2}	12629	87.38 ⁴ F _{5/2} + 8.42 ² H _{9/2} + 2.39 ⁴ F _{7/2}
30	12573	12716	51.76 ⁴ F _{5/2} + 45.13 ² H _{9/2} + 1.43 ⁴ F _{7/2}
31	² H _{9/2}	12846	58.98 ² H _{9/2} + 36.39 ⁴ F _{5/2} + 2.41 ⁴ F _{3/2}
32	12738	12888	61.71 ⁴ F _{5/2} + 34.38 ² H _{9/2} + 1.53 ⁴ F _{7/2}
33		12912	86.46 ² H _{9/2} + 11.78 ⁴ F _{5/2} + 0.84 ⁴ F _{7/2}
34		12999	78.68 ² H _{9/2} + 18.52 ⁴ F _{5/2} + 2.02 ⁴ F _{7/2}
35		13058	89.25 ² H _{9/2} + 9.26 ⁴ F _{5/2} + 0.87 ⁴ F _{7/2}
36		13171	91.52 ² H _{9/2} + 6.89 ⁴ F _{5/2} + 0.72 ⁴ F _{7/2}
37	⁴ S _{3/2}	13643	75.54 ⁴ S _{3/2} + 21.69 ⁴ F _{7/2} + 0.84 ⁴ G _{5/2}
38	13459	13668	48.60 ⁴ S _{3/2} + 47.61 ⁴ F _{7/2} + 1.63 ⁴ F _{5/2}
39	⁴ F _{7/2}	13701	63.83 ⁴ S _{3/2} + 33.45 ⁴ F _{7/2} + 1.10 ⁴ F _{5/2}
40	13564	13731	86.22 ⁴ F _{7/2} + 8.61 ⁴ S _{3/2} + 1.94 ⁴ F _{9/2}
41		13838	92.54 ⁴ F _{7/2} + 3.26 ⁴ F _{9/2} + 1.80 ⁴ F _{5/2}
42		14014	95.38 ⁴ F _{7/2} + 1.42 ⁴ F _{5/2} + 1.22 ⁴ F _{9/2}
43	⁴ F _{9/2}	14930	96.81 ⁴ F _{9/2} + 1.78 ⁴ F _{7/2} + 0.62 ⁴ F _{5/2}
44	14854	14975	98.08 ⁴ F _{9/2} + 0.77 ² H _{11/2} + 0.51 ⁴ F _{7/2}
45		15082	95.06 ⁴ F _{9/2} + 3.20 ⁴ F _{7/2} + 1.04 ² H _{11/2}
46		15266	97.10 ⁴ F _{9/2} + 1.26 ⁴ F _{7/2} + 0.87 ² H _{11/2}
47		15321	97.24 ⁴ F _{9/2} + 1.23 ² H _{11/2} + 0.50 ² G _{7/2}
48	² H _{11/2}	16234	98.87 ² H _{11/2} + 0.52 ² G _{7/2} + 0.46 ⁴ F _{9/2}
49	16043	16260	99.04 ² H _{11/2} + 0.30 ² G _{7/2} + 0.24 ⁴ F _{9/2}
50		16279	98.06 ² H _{11/2} + 0.94 ⁴ F _{9/2} + 0.44 ² G _{7/2}
51		16310	98.56 ² H _{11/2} + 0.64 ⁴ F _{9/2} + 0.37 ² G _{7/2}
52		16336	98.65 ² H _{11/2} + 0.87 ⁴ F _{9/2} + 0.17 ² G _{7/2}
53		16342	98.43 ² H _{11/2} + 0.92 ⁴ F _{9/2} + 0.38 ² G _{7/2}
54	⁴ G _{5/2}	17130	84.61 ⁴ G _{5/2} + 13.55 ² G _{7/2} + 0.54 ⁴ F _{7/2}
55	17167	17357	62.16 ⁴ G _{5/2} + 36.49 ² G _{7/2} + 0.43 ⁴ F _{3/2}
56	² G _{7/2}	17486	56.90 ² G _{7/2} + 41.36 ⁴ G _{5/2} + 0.53 ⁴ F _{9/2}
57	17334	17589	96.54 ² G _{7/2} + 1.94 ⁴ G _{5/2} + 0.63 ² H _{11/2}
58		17682	84.44 ² G _{7/2} + 14.31 ⁴ G _{5/2} + 0.54 ² H _{11/2}
59		17780	66.26 ² G _{7/2} + 32.20 ⁴ G _{5/2} + 0.38 ⁴ S _{3/2}
60		17873	59.11 ⁴ G _{5/2} + 40.05 ² G _{7/2} + 0.24 ⁴ S _{3/2}

^aAqueous centroids (cm⁻¹).

Table 27. Predicted energy levels for Pm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S, L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	5I_4	0	$99.07 ^5I_4 + 0.70 ^5I_5 + 0.18 ^5I_6$
2	Γ_2	99	39	$98.30 ^5I_4 + 1.51 ^5I_5 + 0.12 ^5I_6$
3	Γ_2		190	$97.68 ^5I_4 + 2.08 ^5I_5 + 0.19 ^5I_6$
4	Γ_1		193	$99.36 ^5I_4 + 0.45 ^5I_5 + 0.13 ^5I_6$
5	Γ_2		286	$98.07 ^5I_4 + 1.69 ^5I_5 + 0.14 ^5I_6$
6	Γ_1		325	$98.30 ^5I_4 + 1.42 ^5I_5 + 0.25 ^5I_6$
7	Γ_2		416	$98.53 ^5I_4 + 1.27 ^5I_5 + 0.11 ^5I_6$
8	Γ_1		488	$95.19 ^5I_4 + 4.57 ^5I_5 + 0.18 ^5I_6$
9	Γ_1		560	$97.73 ^5I_4 + 1.94 ^5I_5 + 0.26 ^5I_6$
10	Γ_2	5I_5	1642	$96.36 ^5I_5 + 2.22 ^5I_4 + 1.24 ^5I_6$
11	Γ_1	1577	1645	$97.03 ^5I_5 + 1.92 ^5I_4 + 0.82 ^5I_6$
12	Γ_2		1695	$98.27 ^5I_5 + 0.88 ^5I_4 + 0.57 ^5I_6$
13	Γ_1		1697	$97.27 ^5I_5 + 2.27 ^5I_4 + 0.30 ^5I_6$
14	Γ_2		1742	$97.92 ^5I_5 + 1.34 ^5I_4 + 0.42 ^5I_6$
15	Γ_2		1796	$98.62 ^5I_5 + 0.99 ^5I_6 + 0.28 ^5I_4$
16	Γ_1		1802	$97.10 ^5I_5 + 1.77 ^5I_6 + 1.00 ^5I_4$
17	Γ_1		1813	$95.92 ^5I_5 + 2.44 ^5I_4 + 1.37 ^5I_6$
18	Γ_1		1831	$96.52 ^5I_5 + 1.84 ^5I_6 + 1.43 ^5I_4$
19	Γ_2		1966	$97.21 ^5I_5 + 1.88 ^5I_6 + 0.71 ^5I_4$
20	Γ_2		1972	$97.18 ^5I_5 + 1.53 ^5I_6 + 1.03 ^5I_4$
21	Γ_1	5I_6	3245	$97.78 ^5I_6 + 0.97 ^5I_7 + 0.76 ^5I_5$
22	Γ_2	3186	3259	$96.56 ^5I_6 + 1.77 ^5I_5 + 1.26 ^5I_7$
23	Γ_2		3289	$98.59 ^5I_6 + 0.63 ^5I_5 + 0.47 ^5I_7$
24	Γ_1		3307	$97.86 ^5I_6 + 1.50 ^5I_5 + 0.43 ^5I_7$
25	Γ_2		3344	$97.96 ^5I_6 + 1.46 ^5I_5 + 0.37 ^5I_7$
26	Γ_1		3357	$98.19 ^5I_6 + 0.82 ^5I_5 + 0.65 ^5I_7$
27	Γ_1		3365	$97.02 ^5I_6 + 1.33 ^5I_7 + 1.28 ^5I_5$
28	Γ_2		3424	$98.18 ^5I_6 + 0.91 ^5I_5 + 0.71 ^5I_7$
29	Γ_1		3431	$98.34 ^5I_6 + 0.98 ^5I_7 + 0.44 ^5I_5$
30	Γ_2		3448	$96.48 ^5I_6 + 2.14 ^5I_7 + 1.11 ^5I_5$
31	Γ_2		3455	$97.32 ^5I_6 + 1.93 ^5I_7 + 0.58 ^5I_5$
32	Γ_1		3587	$97.70 ^5I_6 + 1.38 ^5I_7 + 0.67 ^5I_5$
33	Γ_1		3590	$98.01 ^5I_6 + 1.14 ^5I_7 + 0.58 ^5I_5$
34	Γ_2	5I_7	4902	$97.99 ^5I_7 + 0.94 ^5I_6 + 0.68 ^5I_8$
35	Γ_1	4876	4903	$97.29 ^5I_7 + 1.33 ^5I_6 + 1.03 ^5I_8$
36	Γ_2		4971	$98.83 ^5I_7 + 0.54 ^5I_8 + 0.47 ^5I_6$
37	Γ_1		4983	$98.64 ^5I_7 + 0.78 ^5I_8 + 0.40 ^5I_6$
38	Γ_1		4995	$98.21 ^5I_7 + 0.87 ^5I_6 + 0.69 ^5I_8$
39	Γ_2		5013	$97.96 ^5I_7 + 1.29 ^5I_6 + 0.62 ^5I_8$
40	Γ_1		5031	$97.45 ^5I_7 + 1.85 ^5I_6 + 0.59 ^5I_8$
41	Γ_2		5062	$96.60 ^5I_7 + 1.96 ^5I_8 + 1.19 ^5I_6$
42	Γ_2		5076	$97.70 ^5I_7 + 1.10 ^5I_8 + 1.02 ^5I_6$
43	Γ_1		5143	$97.77 ^5I_7 + 1.88 ^5I_8 + 0.15 ^5I_6$
44	Γ_2		5166	$98.46 ^5I_7 + 0.75 ^5I_8 + 0.59 ^5I_6$
45	Γ_1		5185	$96.78 ^5I_7 + 1.95 ^5I_8 + 1.10 ^5I_6$
46	Γ_1		5208	$98.16 ^5I_7 + 1.10 ^5I_6 + 0.63 ^5I_8$
47	Γ_2		5323	$98.17 ^5I_7 + 0.96 ^5I_8 + 0.67 ^5I_6$
48	Γ_2		5325	$98.39 ^5I_7 + 0.80 ^5I_8 + 0.60 ^5I_6$

Table 27 (cont'd).
Predicted energy
levels for Pm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
49	Γ_2	5I_8	6502	$98.61\ ^5I_8 + 1.16\ ^5I_7 + 0.15\ ^5I_6$
50	Γ_1	6611	6506	$98.58\ ^5I_8 + 1.17\ ^5I_7 + 0.15\ ^5I_6$
51	Γ_1		6600	$98.92\ ^5I_8 + 0.95\ ^5I_7 + 0.07\ ^5I_6$
52	Γ_2		6667	$98.24\ ^5I_8 + 1.60\ ^5I_7 + 0.05\ ^5F_5$
53	Γ_1		6674	$99.08\ ^5I_8 + 0.79\ ^5I_7 + 0.07\ ^5I_6$
54	Γ_2		6686	$99.23\ ^5I_8 + 0.66\ ^5I_7 + 0.06\ ^5I_6$
55	Γ_2		6695	$98.53\ ^5I_8 + 1.32\ ^5I_7 + 0.06\ ^5I_6$
56	Γ_1		6769	$99.47\ ^5I_8 + 0.39\ ^5I_7 + 0.06\ ^5F_5$
57	Γ_2		6809	$99.36\ ^5I_8 + 0.45\ ^5I_7 + 0.07\ ^5F_5$
58	Γ_1		6825	$98.95\ ^5I_8 + 0.86\ ^5I_7 + 0.06\ ^5F_4$
59	Γ_1		6921	$97.98\ ^5I_8 + 1.77\ ^5I_7 + 0.11\ ^5F_5$
60	Γ_2		6997	$99.41\ ^5I_8 + 0.35\ ^5I_7 + 0.08\ ^5I_6$
61	Γ_1		7021	$99.21\ ^5I_8 + 0.57\ ^5I_7 + 0.09\ ^5F_5$
62	Γ_2		7068	$98.77\ ^5I_8 + 1.01\ ^5I_7 + 0.12\ ^5F_5$
63	Γ_2		7086	$98.95\ ^5I_8 + 0.81\ ^5I_7 + 0.11\ ^5F_5$
64	Γ_1		7188	$99.35\ ^5I_8 + 0.50\ ^5I_7 + 0.08\ ^5I_6$
65	Γ_1		7191	$99.39\ ^5I_8 + 0.45\ ^5I_7 + 0.08\ ^5I_6$
66	Γ_2	5F_1	12501	$95.17\ ^5F_1 + 2.75\ ^5F_2 + 1.53\ ^5F_3$
67	Γ_2	12397	12523	$89.18\ ^5F_1 + 9.42\ ^5F_2 + 0.99\ ^5F_3$
68	Γ_1		12686	$91.74\ ^5F_1 + 4.60\ ^5F_2 + 3.14\ ^5F_3$
69	Γ_1	5F_2	12799	$95.35\ ^5F_2 + 2.46\ ^5F_1 + 1.66\ ^5F_3$
70	Γ_2	12811	12976	$87.76\ ^5F_2 + 8.84\ ^5F_1 + 1.95\ ^5F_3$
71	Γ_1		12996	$94.54\ ^5F_2 + 2.66\ ^5F_1 + 2.19\ ^5F_3$
72	Γ_1		13069	$97.92\ ^5F_2 + 1.45\ ^5F_4 + 0.27\ ^5F_3$
73	Γ_2		13279	$93.11\ ^5F_2 + 2.99\ ^5F_3 + 2.97\ ^5F_1$
74	Γ_2	5F_3	13727	$96.86\ ^5F_3 + 2.28\ ^5F_4 + 0.31\ ^5F_1$
75	Γ_2	13651	13744	$95.62\ ^5F_3 + 1.89\ ^5F_2 + 1.48\ ^5F_1$
76	Γ_1		13823	$94.53\ ^5F_3 + 2.78\ ^5F_4 + 1.84\ ^5F_2$
77	Γ_2		13827	$93.58\ ^5F_3 + 2.43\ ^5F_2 + 2.33\ ^5F_4$
78	Γ_1		13918	$93.41\ ^5F_3 + 4.35\ ^5F_4 + 1.31\ ^5F_2$
79	Γ_1		13987	$93.14\ ^5F_3 + 2.80\ ^5F_4 + 2.32\ ^5F_1$
80	Γ_2		14074	$96.57\ ^5F_3 + 2.40\ ^5F_4 + 0.45\ ^5F_2$
81	Γ_1	5S_2	14550	$99.78\ ^5S_2 + 0.14\ ^5F_4 + 0.02\ ^5F_3$
82	Γ_2	14337	14552	$99.52\ ^5S_2 + 0.37\ ^5F_4 + 0.04\ ^5F_5$
83	Γ_1		14558	$99.58\ ^5S_2 + 0.27\ ^5F_4 + 0.06\ ^5F_5$
84	Γ_2		14559	$99.87\ ^5S_2 + 0.05\ ^5F_4 + 0.02\ ^5F_3$
85	Γ_1		14561	$99.70\ ^5S_2 + 0.15\ ^5F_4 + 0.06\ ^5F_5$
86	Γ_1	5F_4	14714	$97.60\ ^5F_4 + 1.44\ ^5F_5 + 0.41\ ^5F_2$
87	Γ_2	14561	14728	$94.03\ ^5F_4 + 3.47\ ^5F_5 + 2.00\ ^5F_3$
88	Γ_1		14738	$95.69\ ^5F_4 + 1.92\ ^5F_5 + 1.65\ ^5F_3$
89	Γ_2		14767	$94.20\ ^5F_4 + 2.99\ ^5F_5 + 1.89\ ^5F_3$
90	Γ_1		14793	$93.50\ ^5F_4 + 4.94\ ^5F_3 + 1.16\ ^5F_5$
91	Γ_2		14853	$96.25\ ^5F_4 + 1.46\ ^5F_3 + 1.05\ ^5F_5$
92	Γ_1		14857	$96.12\ ^5F_4 + 3.09\ ^5F_3 + 0.48\ ^5F_5$
93	Γ_1		14865	$97.02\ ^5F_4 + 1.35\ ^5F_2 + 0.98\ ^5F_5$
94	Γ_2		14868	$96.38\ ^5F_4 + 2.53\ ^5F_3 + 0.43\ ^5F_5$
95	Γ_2	5F_5	15865	$98.90\ ^5F_5 + 0.33\ ^3K_6 + 0.27\ ^5F_3$
96	Γ_2	15862	15874	$98.16\ ^5F_5 + 0.90\ ^5F_4 + 0.54\ ^3K_6$
97	Γ_1	3K_6	15929	$96.69\ ^5F_5 + 1.83\ ^3K_6 + 0.91\ ^5F_4$

Table 27 (cont'd).
Predicted energy
levels for Pm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
98	Γ_1	15874	15940	$94.50 {}^5F_5 + 3.20 {}^3K_6 + 1.94 {}^5F_4$
99	Γ_1		16025	$98.68 {}^3K_6 + 1.28 {}^5F_5 + 0.03 {}^5F_4$
100	Γ_1		16026	$97.35 {}^3K_6 + 2.62 {}^5F_5 + 0.01 {}^5F_4$
101	Γ_2		16065	$99.61 {}^3K_6 + 0.36 {}^5F_5 + 0.02 {}^5F_4$
102	Γ_2		16067	$99.09 {}^3K_6 + 0.86 {}^5F_5 + 0.03 {}^5F_3$
103	Γ_1		16079	$98.13 {}^3K_6 + 1.71 {}^5F_5 + 0.14 {}^5F_4$
104	Γ_2		16080	$99.08 {}^3K_6 + 0.83 {}^5F_5 + 0.07 {}^5F_4$
105	Γ_1		16101	$99.02 {}^3K_6 + 0.95 {}^5F_5 + 0.02 {}^5F_3$
106	Γ_1		16101	$99.16 {}^3K_6 + 0.79 {}^5F_5 + 0.03 {}^5F_4$
107	Γ_2		16111	$90.74 {}^3K_6 + 9.06 {}^5F_5 + 0.17 {}^5F_4$
108	Γ_2		16120	$94.40 {}^3K_6 + 5.39 {}^5F_5 + 0.18 {}^5F_4$
109	Γ_1		16120	$99.45 {}^3K_6 + 0.52 {}^5F_5 + 0.02 {}^5F_3$
110	Γ_2		16135	$75.39 {}^3K_6 + 23.65 {}^5F_5 + 0.88 {}^5F_4$
111	Γ_1		16143	$98.92 {}^3K_6 + 1.00 {}^5F_5 + 0.04 {}^5F_4$
112	Γ_2		16151	$61.89 {}^5F_5 + 36.02 {}^3K_6 + 1.90 {}^5F_4$
113	Γ_1		16173	$96.43 {}^5F_5 + 1.88 {}^3K_6 + 1.44 {}^5F_4$
114	Γ_2		16210	$96.73 {}^5F_5 + 2.13 {}^5F_4 + 0.70 {}^3K_6$
115	Γ_1		16218	$97.04 {}^5F_5 + 1.59 {}^3K_6 + 1.07 {}^5F_4$
116	Γ_2		16238	$95.27 {}^5F_5 + 3.55 {}^3K_6 + 0.88 {}^5F_4$
117	Γ_2	16347	16347	$98.48 {}^5F_5 + 0.70 {}^5F_4 + 0.35 {}^5F_3$
118	Γ_1		16349	$98.24 {}^5F_5 + 0.79 {}^5F_4 + 0.50 {}^3K_6$

^aAqueous centroids (cm^{-1}).

Table 28. Predicted
energy levels for
 Sm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$,
 C_s site. B_{nm} from table
9.

Level	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	${}^6H_{5/2}$	0	$96.70 {}^6H_{5/2} + 2.54 {}^6H_{7/2} + 0.25 {}^6H_{9/2}$
2	46	241	$94.54 {}^6H_{5/2} + 4.17 {}^6H_{7/2} + 0.84 {}^6H_{9/2}$
3		509	$87.61 {}^6H_{5/2} + 11.24 {}^6H_{7/2} + 0.84 {}^6H_{9/2}$
4	${}^6H_{7/2}$	1135	$93.83 {}^6H_{7/2} + 2.71 {}^6H_{9/2} + 2.62 {}^6H_{5/2}$
5	1084	1241	$93.81 {}^6H_{7/2} + 3.25 {}^6H_{5/2} + 1.81 {}^6H_{9/2}$
6		1472	$84.91 {}^6H_{7/2} + 8.89 {}^6H_{5/2} + 5.16 {}^6H_{9/2}$
7		1580	$91.58 {}^6H_{7/2} + 5.47 {}^6H_{9/2} + 2.19 {}^6H_{5/2}$
8	${}^6H_{9/2}$	2349	$94.81 {}^6H_{9/2} + 2.32 {}^6H_{11/2} + 1.62 {}^6H_{7/2}$
9	2299	2449	$94.72 {}^6H_{9/2} + 2.58 {}^6H_{7/2} + 1.35 {}^6H_{11/2}$
10		2549	$90.37 {}^6H_{9/2} + 3.81 {}^6H_{11/2} + 3.50 {}^6H_{7/2}$
11		2712	$90.04 {}^6H_{9/2} + 4.29 {}^6H_{11/2} + 4.14 {}^6H_{7/2}$
12		2811	$93.46 {}^6H_{9/2} + 4.06 {}^6H_{11/2} + 1.59 {}^6H_{7/2}$
13	${}^6H_{11/2}$	3653	$94.84 {}^6H_{11/2} + 2.06 {}^6H_{13/2} + 1.51 {}^6H_{9/2}$
14	3638	3783	$95.60 {}^6H_{11/2} + 1.67 {}^6H_{13/2} + 1.29 {}^6H_{9/2}$
15		3855	$91.64 {}^6H_{11/2} + 4.08 {}^6H_{9/2} + 2.53 {}^6H_{13/2}$
16		3925	$92.37 {}^6H_{11/2} + 2.79 {}^6H_{9/2} + 2.78 {}^6H_{13/2}$
17		4065	$90.51 {}^6H_{11/2} + 4.70 {}^6H_{13/2} + 3.56 {}^6H_{9/2}$
18		4181	$93.36 {}^6H_{11/2} + 4.79 {}^6H_{13/2} + 1.04 {}^6H_{9/2}$
19	${}^6H_{13/2}$	4984	$95.39 {}^6H_{13/2} + 1.31 {}^6H_{15/2} + 1.16 {}^6H_{11/2}$
20	5060	5178	$92.68 {}^6H_{13/2} + 2.63 {}^6H_{15/2} + 2.42 {}^6H_{11/2}$
21		5257	$93.16 {}^6H_{13/2} + 3.69 {}^6H_{11/2} + 1.35 {}^6H_{15/2}$
22		5300	$95.00 {}^6H_{13/2} + 2.21 {}^6H_{15/2} + 1.39 {}^6H_{11/2}$
23		5385	$92.31 {}^6H_{13/2} + 3.22 {}^6H_{11/2} + 2.72 {}^6H_{15/2}$
24		5513	$88.78 {}^6H_{13/2} + 5.21 {}^6H_{15/2} + 4.42 {}^6H_{11/2}$
25		5715	$94.47 {}^6H_{13/2} + 3.61 {}^6H_{15/2} + 0.94 {}^6H_{11/2}$

Table 28 (cont'd).
Predicted energy
levels for Sm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
26	${}^6F_{1/2}$	6326	$96.32 {}^6H_{15/2} + 0.96 {}^6F_{9/2} + 0.82 {}^6H_{13/2}$
27	6422	6467	$95.39 {}^6H_{15/2} + 1.83 {}^6H_{13/2} + 0.96 {}^6F_{11/2}$
28	${}^6H_{15/2}$ 6531	6657	$92.85 {}^6H_{15/2} + 2.79 {}^6H_{13/2} + 1.82 {}^6F_{3/2}$
29	${}^6F_{3/2}$	6698	$94.05 {}^6H_{15/2} + 3.04 {}^6H_{13/2} + 0.86 {}^6F_{7/2}$
30	6666	6744	$87.21 {}^6F_{1/2} + 7.87 {}^6F_{3/2} + 1.47 {}^6H_{15/2}$
31		6859	$91.58 {}^6H_{15/2} + 3.42 {}^6F_{3/2} + 2.57 {}^6H_{13/2}$
32		6972	$83.31 {}^6H_{15/2} + 11.40 {}^6F_{3/2} + 1.79 {}^6H_{13/2}$
33		7004	$72.34 {}^6F_{3/2} + 13.91 {}^6H_{15/2} + 6.51 {}^6F_{5/2}$
34		7038	$88.44 {}^6F_{3/2} + 3.64 {}^6F_{1/2} + 3.44 {}^6H_{15/2}$
35		7173	$91.25 {}^6H_{15/2} + 3.28 {}^6H_{13/2} + 2.92 {}^6F_{5/2}$
36		7437	$89.08 {}^6H_{15/2} + 7.35 {}^6F_{5/2} + 1.27 {}^6F_{7/2}$
37	${}^6F_{5/2}$	7471	$89.61 {}^6F_{5/2} + 6.62 {}^6H_{15/2} + 0.84 {}^6F_{3/2}$
38	7158	7552	$89.25 {}^6F_{5/2} + 4.09 {}^6H_{15/2} + 3.14 {}^6F_{3/2}$
39		7618	$90.01 {}^6F_{5/2} + 4.67 {}^6F_{3/2} + 1.87 {}^6H_{15/2}$
40	${}^6F_{7/2}$	8303	$96.12 {}^6F_{7/2} + 1.77 {}^6H_{15/2} + 0.66 {}^6H_{13/2}$
41	8006	8327	$96.74 {}^6F_{7/2} + 0.66 {}^6F_{9/2} + 0.63 {}^6H_{13/2}$
42		8416	$95.05 {}^6F_{7/2} + 1.35 {}^6F_{5/2} + 1.12 {}^6H_{15/2}$
43		8495	$95.54 {}^6F_{7/2} + 1.53 {}^6H_{15/2} + 0.65 {}^6H_{13/2}$
44	${}^6F_{9/2}$	9418	$97.78 {}^6F_{9/2} + 1.18 {}^6H_{15/2} + 0.43 {}^6F_{7/2}$
45	9167	9506	$96.60 {}^6F_{9/2} + 1.31 {}^6F_{11/2} + 0.67 {}^6H_{15/2}$
46		9541	$95.80 {}^6F_{9/2} + 1.92 {}^6F_{11/2} + 0.68 {}^6H_{15/2}$
47		9604	$97.44 {}^6F_{9/2} + 1.10 {}^6H_{15/2} + 0.38 {}^6H_{13/2}$
48		9630	$97.11 {}^6F_{9/2} + 0.94 {}^6H_{15/2} + 0.64 {}^6F_{7/2}$
49	${}^6F_{11/2}$	10742	$98.57 {}^6F_{11/2} + 0.77 {}^6H_{15/2} + 0.26 {}^6F_{9/2}$
50	10552	10798	$98.51 {}^6F_{11/2} + 0.42 {}^6H_{13/2} + 0.41 {}^6H_{15/2}$
51		10943	$97.43 {}^6F_{11/2} + 1.12 {}^6F_{9/2} + 0.92 {}^6H_{15/2}$
52		10980	$98.80 {}^6F_{11/2} + 0.48 {}^6F_{9/2} + 0.42 {}^6H_{15/2}$
53		10988	$97.76 {}^6F_{11/2} + 1.08 {}^6F_{9/2} + 0.70 {}^6H_{15/2}$
54		11125	$97.37 {}^6F_{11/2} + 1.78 {}^6H_{15/2} + 0.33 {}^6H_{13/2}$
55	${}^4G_{5/2}$	17857	$98.44 {}^4G_{5/2} + 1.55 {}^4F_{3/2}$
56	17935	18234	$97.84 {}^4G_{5/2} + 2.16 {}^4F_{3/2}$
57		18597	$98.86 {}^4G_{5/2} + 1.14 {}^4F_{3/2}$
58	${}^4F_{3/2}$	19211	$98.18 {}^4F_{3/2} + 1.82 {}^4G_{5/2}$
59	18899	19261	$96.97 {}^4F_{3/2} + 3.03 {}^4G_{5/2}$

^aAqueous centroids (cm^{-1}).

Table 29. Predicted
energy levels for Eu^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	7F_0	0	$91.81 {}^7F_0 + 6.51 {}^7F_2 + 1.56 {}^7F_4$
2	Γ_2	7F_1	252	$95.54 {}^7F_1 + 1.82 {}^7F_3 + 1.35 {}^7F_2$
3	Γ_2	354	288	$92.28 {}^7F_1 + 3.93 {}^7F_3 + 2.71 {}^7F_2$
4	Γ_1		670	$89.80 {}^7F_1 + 5.46 {}^7F_3 + 3.44 {}^7F_2$
5	Γ_1	7F_2	819	$91.25 {}^7F_2 + 5.93 {}^7F_3 + 1.49 {}^7F_1$
6	Γ_1	1018	919	$85.02 {}^7F_2 + 11.01 {}^7F_3 + 2.49 {}^7F_1$
7	Γ_2		1065	$93.35 {}^7F_2 + 2.66 {}^7F_1 + 1.51 {}^7F_5$
8	Γ_1		1258	$87.02 {}^7F_2 + 5.12 {}^7F_0 + 4.73 {}^7F_3$
9	Γ_2		1384	$80.73 {}^7F_2 + 16.47 {}^7F_3 + 1.67 {}^7F_4$

Table 29 (cont'd).
Predicted energy
levels for Eu³⁺ in
Ca₅(PO₄)₃F, C_s site.
B_{nm} from table 9.

Level	I. R.	[(S,L)] ^a	Energy (cm ⁻¹)	Free ion mixture (%)
10	Γ ₂	⁷ F ₃	1823	91.05 ⁷ F ₃ + 6.67 ⁷ F ₄ + 1.06 ⁷ F ₅
11	Γ ₂	1881	1911	77.28 ⁷ F ₃ + 12.51 ⁷ F ₂ + 8.94 ⁷ F ₄
12	Γ ₁		1963	79.43 ⁷ F ₃ + 10.43 ⁷ F ₄ + 8.37 ⁷ F ₂
13	Γ ₁		2077	90.54 ⁷ F ₃ + 3.54 ⁷ F ₁ + 3.31 ⁷ F ₅
14	Γ ₂		2085	90.82 ⁷ F ₃ + 3.93 ⁷ F ₂ + 3.50 ⁷ F ₅
15	Γ ₁		2114	74.11 ⁷ F ₃ + 13.83 ⁷ F ₄ + 9.92 ⁷ F ₂
16	Γ ₂		2133	89.66 ⁷ F ₃ + 5.35 ⁷ F ₁ + 3.97 ⁷ F ₄
17	Γ ₁	⁷ F ₄	2764	84.91 ⁷ F ₄ + 8.45 ⁷ F ₃ + 3.21 ⁷ F ₅
18	Γ ₂	2867	2772	94.17 ⁷ F ₄ + 2.44 ⁷ F ₅ + 1.30 ⁷ F ₃
19	Γ ₂		2934	84.96 ⁷ F ₄ + 7.07 ⁷ F ₅ + 4.85 ⁷ F ₃
20	Γ ₁		2937	78.74 ⁷ F ₄ + 12.21 ⁷ F ₃ + 5.82 ⁷ F ₅
21	Γ ₁		3091	92.30 ⁷ F ₄ + 3.22 ⁷ F ₅ + 2.53 ⁷ F ₆
22	Γ ₂		3101	84.81 ⁷ F ₄ + 8.81 ⁷ F ₃ + 4.55 ⁷ F ₅
23	Γ ₁		3174	88.56 ⁷ F ₄ + 8.03 ⁷ F ₅ + 1.71 ⁷ F ₆
24	Γ ₁		3208	90.44 ⁷ F ₄ + 4.77 ⁷ F ₅ + 2.08 ⁷ F ₆
25	Γ ₂		3230	87.37 ⁷ F ₄ + 5.89 ⁷ F ₅ + 3.79 ⁷ F ₃
26	Γ ₁	⁷ F ₅	3858	86.02 ⁷ F ₅ + 10.09 ⁷ F ₆ + 2.71 ⁷ F ₄
27	Γ ₂	3928	3875	83.05 ⁷ F ₅ + 10.16 ⁷ F ₆ + 4.50 ⁷ F ₄
28	Γ ₂		3892	85.02 ⁷ F ₅ + 8.73 ⁷ F ₆ + 4.88 ⁷ F ₄
29	Γ ₁		3921	86.95 ⁷ F ₅ + 7.19 ⁷ F ₆ + 4.83 ⁷ F ₄
30	Γ ₂		3977	89.33 ⁷ F ₅ + 7.54 ⁷ F ₆ + 2.00 ⁷ F ₄
31	Γ ₁		3986	87.03 ⁷ F ₅ + 8.56 ⁷ F ₆ + 1.86 ⁷ F ₃
32	Γ ₂		4121	90.83 ⁷ F ₅ + 3.05 ⁷ F ₆ + 2.99 ⁷ F ₃
33	Γ ₁		4148	83.94 ⁷ F ₅ + 7.83 ⁷ F ₆ + 7.14 ⁷ F ₄
34	Γ ₁		4290	86.19 ⁷ F ₅ + 7.86 ⁷ F ₆ + 4.44 ⁷ F ₄
35	Γ ₂		4437	93.69 ⁷ F ₅ + 4.60 ⁷ F ₆ + 0.88 ⁷ F ₄
36	Γ ₂		4463	95.34 ⁷ F ₅ + 2.57 ⁷ F ₆ + 1.47 ⁷ F ₄
37	Γ ₁	⁷ F ₆	4908	91.27 ⁷ F ₆ + 4.38 ⁷ F ₅ + 3.66 ⁷ F ₄
38	Γ ₂	5029	4908	90.66 ⁷ F ₆ + 4.84 ⁷ F ₅ + 3.92 ⁷ F ₄
39	Γ ₁		4951	96.59 ⁷ F ₆ + 1.72 ⁷ F ₅ + 1.47 ⁷ F ₄
40	Γ ₂		4955	95.71 ⁷ F ₆ + 2.96 ⁷ F ₅ + 0.88 ⁷ F ₄
41	Γ ₁		5162	90.70 ⁷ F ₆ + 6.69 ⁷ F ₅ + 1.99 ⁷ F ₄
42	Γ ₂		5201	90.80 ⁷ F ₆ + 7.80 ⁷ F ₅ + 0.79 ⁷ F ₄
43	Γ ₂		5321	85.27 ⁷ F ₆ + 13.49 ⁷ F ₅ + 0.94 ⁷ F ₄
44	Γ ₁		5409	89.29 ⁷ F ₆ + 9.68 ⁷ F ₅ + 0.91 ⁷ F ₄
45	Γ ₁		5447	86.94 ⁷ F ₆ + 12.83 ⁷ F ₅ + 0.14 ⁷ F ₄
46	Γ ₂		5611	96.66 ⁷ F ₆ + 2.63 ⁷ F ₅ + 0.47 ⁷ F ₄
47	Γ ₂		5617	96.53 ⁷ F ₆ + 2.83 ⁷ F ₅ + 0.37 ⁷ F ₄
48	Γ ₁		5719	98.33 ⁷ F ₆ + 1.05 ⁷ F ₅ + 0.54 ⁷ F ₄
49	Γ ₁		5720	98.42 ⁷ F ₆ + 0.95 ⁷ F ₅ + 0.55 ⁷ F ₄
50	Γ ₁	⁵ D ₀ 17286	17447	99.89 ⁵ D ₀ + 0.06 ⁵ D ₂ + 0.05 ⁵ L ₆
51	Γ ₂	⁵ D ₁	19135	99.91 ⁵ D ₁ + 0.05 ⁵ D ₂ + 0.03 ⁵ D ₃
52	Γ ₂	19026	19167	99.89 ⁵ D ₁ + 0.09 ⁵ D ₂ + 0.02 ⁵ L ₆
53	Γ ₁		19270	99.94 ⁵ D ₁ + 0.04 ⁵ D ₃ + 0.02 ⁵ L ₆
54	Γ ₂	⁵ D ₂	21619	99.78 ⁵ D ₂ + 0.13 ⁵ D ₃ + 0.05 ⁵ D ₁
55	Γ ₁	21499	21626	99.85 ⁵ D ₂ + 0.10 ⁵ D ₃ + 0.03 ⁵ L ₆
56	Γ ₁		21649	99.81 ⁵ D ₂ + 0.14 ⁵ D ₃ + 0.03 ⁵ L ₆
57	Γ ₂		21696	99.77 ⁵ D ₂ + 0.10 ⁵ D ₃ + 0.09 ⁵ D ₁
58	Γ ₁		21728	99.94 ⁵ D ₂ + 0.03 ⁵ D ₀ + 0.02 ⁵ L ₆

Table 29 (cont'd).
Predicted energy
levels for Eu^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
59	Γ_1	5D_3 24390	24504	$99.87 ^5D_3 + 0.06 ^5D_2 + 0.04 ^5L_6$
60	Γ_2		24514	$99.85 ^5D_3 + 0.09 ^5D_2 + 0.03 ^5L_6$
61	Γ_2		24523	$99.88 ^5D_3 + 0.10 ^5D_2 + 0.02 ^5L_6$
62	Γ_1		24560	$99.87 ^5D_3 + 0.07 ^5L_6 + 0.06 ^5D_2$
63	Γ_1		24581	$99.83 ^5D_3 + 0.13 ^5D_2 + 0.04 ^5L_6$
64	Γ_2	5L_6 25375	24610	$99.92 ^5D_3 + 0.04 ^5L_6 + 0.04 ^5D_2$
65	Γ_2		24626	$99.96 ^5D_3 + 0.03 ^5L_6 + 0.01 ^5D_1$
66	Γ_1		25171	$99.90 ^5L_6 + 0.06 ^5D_3 + 0.02 ^5D_2$
67	Γ_2		25201	$99.93 ^5L_6 + 0.04 ^5D_3 + 0.02 ^5D_2$
68	Γ_1		25214	$99.93 ^5L_6 + 0.04 ^5D_3 + 0.02 ^5D_2$
69	Γ_2		25246	$99.96 ^5L_6 + 0.01 ^5D_2 + 0.01 ^5D_3$
70	Γ_2		25407	$99.96 ^5L_6 + 0.02 ^5D_3 + 0.01 ^5D_2$
71	Γ_1		25436	$99.96 ^5L_6 + 0.03 ^5D_3 + 0.01 ^5D_2$
72	Γ_1		25509	$99.98 ^5L_6 + 0.01 ^5D_0 + 0.01 ^5D_2$
73	Γ_2		25656	$99.96 ^5L_6 + 0.02 ^5D_3 + 0.01 ^5D_2$
74	Γ_2		25718	$99.98 ^5L_6 + 0.01 ^5D_2 + 0.01 ^5D_3$
75	Γ_1		25835	$99.98 ^5L_6 + 0.01 ^5D_0 + 0.01 ^5D_3$
76	Γ_1		25856	$99.98 ^5L_6 + 0.01 ^5D_2$
77	Γ_1		25908	$99.97 ^5L_6 + 0.02 ^5D_2 + 0.01 ^5D_3$
78	Γ_2		25915	$99.96 ^5L_6 + 0.02 ^5D_3 + 0.02 ^5D_2$

^aAqueous centroids (cm^{-1}).

Table 30. Predicted
energy levels for Gd^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	$^8S_{7/2}$	0	$100.00 ^8S_{7/2}$
2	14	0.3	$100.00 ^8S_{7/2}$
3		0.8	$100.00 ^8S_{7/2}$
4		1.4	$100.00 ^8S_{7/2}$
5	$^6P_{7/2}$	32074	$99.44 ^6P_{7/2} + 0.15 ^6P_{3/2} + 0.09 ^6P_{5/2}$
6	32224	32127	$98.84 ^6P_{7/2} + 0.69 ^6P_{5/2} + 0.15 ^6P_{3/2}$
7		32217	$98.59 ^6P_{7/2} + 1.06 ^6P_{5/2} + 0.07 ^6I_{13/2}$
8		32340	$99.54 ^6P_{7/2} + 0.08 ^6I_{17/2} + 0.06 ^6I_{11/2}$
9		32661	$98.30 ^6P_{5/2} + 0.78 ^6P_{3/2} + 0.40 ^6P_{7/2}$
10	32767	32706	$95.08 ^6P_{5/2} + 3.74 ^6P_{3/2} + 0.73 ^6P_{7/2}$
11		32815	$98.55 ^6P_{5/2} + 0.82 ^6P_{7/2} + 0.16 ^6I_{17/2}$
12		33247	$95.61 ^6P_{3/2} + 3.74 ^6P_{5/2} + 0.13 ^6I_{13/2}$
13	33303	33319	$98.30 ^6P_{3/2} + 1.01 ^6P_{5/2} + 0.14 ^6I_{13/2}$
14	$^6I_{7/2}$	35823	$99.54 ^6I_{7/2} + 0.21 ^6I_{9/2} + 0.13 ^6P_{5/2}$
15	35879	35841	$99.77 ^6I_{7/2} + 0.17 ^6I_{9/2} + 0.01 ^6P_{7/2}$
16		35890	$99.49 ^6I_{7/2} + 0.28 ^6I_{9/2} + 0.13 ^6P_{5/2}$
17		35917	$99.52 ^6I_{7/2} + 0.24 ^6I_{9/2} + 0.13 ^6P_{5/2}$
18		36164	$99.09 ^6I_{9/2} + 0.28 ^6I_{11/2} + 0.18 ^6I_{13/2}$
19	36231	36185	$99.36 ^6I_{9/2} + 0.30 ^6I_{11/2} + 0.17 ^6I_{7/2}$
20		36206	$98.77 ^6I_{9/2} + 0.64 ^6I_{11/2} + 0.22 ^6I_{7/2}$
21		36261	$98.95 ^6I_{9/2} + 0.42 ^6I_{11/2} + 0.18 ^6I_{7/2}$
22		36278	$98.77 ^6I_{9/2} + 0.58 ^6I_{11/2} + 0.15 ^6I_{15/2}$

Table 30 (cont'd).
Predicted energy
levels for Gd³⁺ in
Ca₅(PO₄)₃F, C_s site.
B_{nm} from table 9.

Level	[(S,L)] ^a	Energy (cm ⁻¹)	Free ion mixture (%)
23	⁶ I _{17/2}	36433	67.66 ⁶ I _{17/2} + 29.81 ⁶ I _{11/2} + 1.19 ⁶ I _{15/2}
24	36462	36441	86.79 ⁶ I _{17/2} + 10.77 ⁶ I _{11/2} + 1.35 ⁶ I _{13/2}
25		36443	93.57 ⁶ I _{17/2} + 3.69 ⁶ I _{11/2} + 2.05 ⁶ I _{15/2}
26		36444	96.25 ⁶ I _{17/2} + 2.07 ⁶ I _{11/2} + 1.40 ⁶ I _{15/2}
27		36445	94.20 ⁶ I _{17/2} + 4.08 ⁶ I _{11/2} + 0.91 ⁶ I _{15/2}
28		36446	97.16 ⁶ I _{17/2} + 1.66 ⁶ I _{15/2} + 0.53 ⁶ I _{11/2}
29		36447	96.36 ⁶ I _{17/2} + 2.46 ⁶ I _{11/2} + 0.61 ⁶ I _{13/2}
30		36449	93.64 ⁶ I _{17/2} + 4.81 ⁶ I _{11/2} + 0.90 ⁶ I _{15/2}
31		36450	97.62 ⁶ I _{17/2} + 0.96 ⁶ I _{11/2} + 0.74 ⁶ I _{15/2}
32	⁶ I _{11/2}	36459	54.77 ⁶ I _{11/2} + 42.19 ⁶ I _{17/2} + 2.43 ⁶ I _{15/2}
33	36526	36478	95.57 ⁶ I _{11/2} + 3.00 ⁶ I _{17/2} + 0.71 ⁶ I _{13/2}
34		36495	91.18 ⁶ I _{11/2} + 6.30 ⁶ I _{17/2} + 1.53 ⁶ I _{13/2}
35		36514	92.91 ⁶ I _{11/2} + 4.95 ⁶ I _{17/2} + 0.89 ⁶ I _{13/2}
36		36567	95.23 ⁶ I _{11/2} + 1.54 ⁶ I _{13/2} + 1.41 ⁶ I _{17/2}
37		36579	94.45 ⁶ I _{11/2} + 2.05 ⁶ I _{15/2} + 1.71 ⁶ I _{17/2}
38	⁶ I _{13/2}	36636	92.62 ⁶ I _{13/2} + 3.89 ⁶ I _{15/2} + 2.32 ⁶ I _{17/2}
39	36711	36655	71.13 ⁶ I _{13/2} + 25.86 ⁶ I _{15/2} + 1.98 ⁶ I _{11/2}
40	⁶ I _{15/2}	36658	55.23 ⁶ I _{13/2} + 42.27 ⁶ I _{15/2} + 1.44 ⁶ I _{11/2}
41	36725	36663	76.12 ⁶ I _{15/2} + 19.74 ⁶ I _{13/2} + 2.59 ⁶ I _{17/2}
42		36689	63.95 ⁶ I _{13/2} + 34.61 ⁶ I _{15/2} + 0.77 ⁶ I _{17/2}
43		36696	64.41 ⁶ I _{15/2} + 34.09 ⁶ I _{13/2} + 0.74 ⁶ I _{17/2}
44		36701	60.46 ⁶ I _{13/2} + 38.14 ⁶ I _{15/2} + 0.73 ⁶ I _{17/2}
45		36709	62.26 ⁶ I _{15/2} + 35.63 ⁶ I _{13/2} + 1.18 ⁶ I _{11/2}
46		36714	82.56 ⁶ I _{15/2} + 15.83 ⁶ I _{13/2} + 0.80 ⁶ I _{17/2}
47		36723	71.72 ⁶ I _{15/2} + 26.08 ⁶ I _{13/2} + 1.27 ⁶ I _{11/2}
48		36731	71.83 ⁶ I _{15/2} + 26.57 ⁶ I _{13/2} + 0.88 ⁶ I _{17/2}
49		36753	52.22 ⁶ I _{13/2} + 45.77 ⁶ I _{15/2} + 1.16 ⁶ I _{17/2}
50		36756	50.26 ⁶ I _{13/2} + 47.79 ⁶ I _{15/2} + 1.15 ⁶ I _{11/2}
51		36793	61.83 ⁶ I _{15/2} + 36.53 ⁶ I _{13/2} + 1.02 ⁶ I _{17/2}
52		36793	52.08 ⁶ I _{15/2} + 46.12 ⁶ I _{13/2} + 1.26 ⁶ I _{17/2}
53	⁶ D _{9/2}	39617	99.01 ⁶ D _{9/2} + 0.50 ⁶ D _{7/2} + 0.18 ⁶ D _{1/2}
54	39779	39672	98.50 ⁶ D _{9/2} + 1.08 ⁶ D _{7/2} + 0.12 ⁶ D _{1/2}
55		39776	98.44 ⁶ D _{9/2} + 1.31 ⁶ D _{7/2} + 0.06 ⁶ D _{5/2}
56		39809	99.39 ⁶ D _{9/2} + 0.31 ⁶ D _{7/2} + 0.07 ⁶ P _{5/2}
57		39947	99.09 ⁶ D _{9/2} + 0.43 ⁶ D _{7/2} + 0.26 ⁶ D _{1/2}
58	⁶ D _{1/2}	40553	73.98 ⁶ D _{1/2} + 11.90 ⁶ D _{7/2} + 8.71 ⁶ D _{3/2}
59	40621	40661	70.51 ⁶ D _{7/2} + 22.33 ⁶ D _{3/2} + 4.19 ⁶ D _{1/2}
60	⁶ D _{7/2}	40691	87.94 ⁶ D _{7/2} + 5.82 ⁶ D _{3/2} + 3.87 ⁶ D _{5/2}
61	40713	40710	94.21 ⁶ D _{7/2} + 3.45 ⁶ D _{5/2} + 1.14 ⁶ D _{1/2}
62		40719	82.47 ⁶ D _{7/2} + 9.30 ⁶ D _{1/2} + 4.21 ⁶ D _{5/2}
63	⁶ D _{3/2}	40795	63.05 ⁶ D _{3/2} + 22.15 ⁶ D _{7/2} + 13.44 ⁶ D _{5/2}
64	40851	40892	58.96 ⁶ D _{5/2} + 33.16 ⁶ D _{3/2} + 6.37 ⁶ D _{7/2}
65	⁶ D _{5/2}	40955	47.55 ⁶ D _{5/2} + 36.75 ⁶ D _{3/2} + 11.35 ⁶ D _{7/2}
66	40978	41028	73.36 ⁶ D _{5/2} + 17.28 ⁶ D _{3/2} + 6.71 ⁶ D _{7/2}
67		41082	87.80 ⁶ D _{5/2} + 8.73 ⁶ D _{3/2} + 2.17 ⁶ D _{7/2}

^aAqueous centroids (cm⁻¹).

Table 31. Predicted energy levels for Tb³⁺ in Ca₅(PO₄)₃F, C_s site. B_{nm} from table 9.

Level	I. R.	[(S,L)] ^a	Energy (cm ⁻¹)	Free ion mixture (%)
1	Γ ₁	⁷ F ₆	0	99.38 ⁷ F ₆ + 0.30 ⁷ F ₅ + 0.27 ⁷ F ₄
2	Γ ₁	74	1	99.34 ⁷ F ₆ + 0.37 ⁷ F ₅ + 0.25 ⁷ F ₄
3	Γ ₂		119	98.84 ⁷ F ₆ + 0.83 ⁷ F ₅ + 0.20 ⁷ F ₄
4	Γ ₂		124	98.78 ⁷ F ₆ + 0.92 ⁷ F ₅ + 0.16 ⁷ F ₄
5	Γ ₁		340	95.55 ⁷ F ₆ + 4.25 ⁷ F ₅ + 0.15 ⁷ F ₄
6	Γ ₁		362	96.10 ⁷ F ₆ + 3.51 ⁷ F ₅ + 0.32 ⁷ F ₄
7	Γ ₂		481	94.84 ⁷ F ₆ + 4.68 ⁷ F ₅ + 0.30 ⁷ F ₄
8	Γ ₂		557	96.99 ⁷ F ₆ + 2.43 ⁷ F ₅ + 0.30 ⁷ F ₄
9	Γ ₁		604	96.75 ⁷ F ₆ + 2.19 ⁷ F ₅ + 0.75 ⁷ F ₄
10	Γ ₁		768	99.21 ⁷ F ₆ + 0.35 ⁷ F ₅ + 0.31 ⁷ F ₄
11	Γ ₂		770	99.19 ⁷ F ₆ + 0.35 ⁷ F ₅ + 0.26 ⁷ F ₄
12	Γ ₁		841	97.36 ⁷ F ₆ + 1.25 ⁷ F ₄ + 1.15 ⁷ F ₅
13	Γ ₂		841	97.33 ⁷ F ₆ + 1.28 ⁷ F ₄ + 1.17 ⁷ F ₅
14	Γ ₂	⁷ F ₅	2181	97.81 ⁷ F ₅ + 0.92 ⁷ F ₄ + 0.75 ⁷ F ₆
15	Γ ₂	2112	2198	97.71 ⁷ F ₅ + 0.96 ⁷ F ₄ + 0.82 ⁷ F ₆
16	Γ ₁		2355	92.56 ⁷ F ₅ + 5.07 ⁷ F ₄ + 1.22 ⁷ F ₆
17	Γ ₁		2460	91.22 ⁷ F ₅ + 5.29 ⁷ F ₄ + 2.66 ⁷ F ₆
18	Γ ₂		2507	94.33 ⁷ F ₅ + 1.94 ⁷ F ₃ + 1.76 ⁷ F ₆
19	Γ ₁		2584	91.93 ⁷ F ₅ + 4.50 ⁷ F ₆ + 2.28 ⁷ F ₄
20	Γ ₂		2617	93.75 ⁷ F ₅ + 2.63 ⁷ F ₆ + 2.63 ⁷ F ₄
21	Γ ₂		2678	91.44 ⁷ F ₅ + 3.84 ⁷ F ₆ + 3.54 ⁷ F ₄
22	Γ ₁		2696	94.16 ⁷ F ₅ + 2.79 ⁷ F ₄ + 1.57 ⁷ F ₆
23	Γ ₁		2726	94.74 ⁷ F ₅ + 2.06 ⁷ F ₆ + 1.79 ⁷ F ₄
24	Γ ₂		2735	94.39 ⁷ F ₅ + 2.66 ⁷ F ₄ + 1.21 ⁷ F ₃
25	Γ ₂	⁷ F ₄	3595	90.69 ⁷ F ₄ + 3.75 ⁷ F ₃ + 3.38 ⁷ F ₅
26	Γ ₁	3370	3616	93.49 ⁷ F ₄ + 3.05 ⁷ F ₅ + 1.14 ⁷ F ₃
27	Γ ₁		3641	92.09 ⁷ F ₄ + 5.24 ⁷ F ₅ + 1.30 ⁷ F ₀
28	Γ ₁		3719	94.35 ⁷ F ₄ + 2.56 ⁷ F ₅ + 1.67 ⁷ F ₂
29	Γ ₂		3726	86.45 ⁷ F ₄ + 8.65 ⁷ F ₃ + 3.18 ⁷ F ₅
30	Γ ₂		3857	87.56 ⁷ F ₄ + 5.63 ⁷ F ₃ + 5.31 ⁷ F ₅
31	Γ ₁		3869	82.10 ⁷ F ₄ + 11.45 ⁷ F ₃ + 3.81 ⁷ F ₅
32	Γ ₁		4027	86.42 ⁷ F ₄ + 8.24 ⁷ F ₃ + 2.53 ⁷ F ₅
33	Γ ₂		4029	94.90 ⁷ F ₄ + 1.79 ⁷ F ₅ + 1.61 ⁷ F ₂
34	Γ ₂	⁷ F ₃	4666	87.52 ⁷ F ₃ + 7.88 ⁷ F ₁ + 3.97 ⁷ F ₄
35	Γ ₁	4344	4682	75.22 ⁷ F ₃ + 10.30 ⁷ F ₂ + 9.27 ⁷ F ₄
36	Γ ₂		4708	86.98 ⁷ F ₃ + 8.53 ⁷ F ₂ + 2.75 ⁷ F ₅
37	Γ ₁		4714	85.77 ⁷ F ₃ + 5.43 ⁷ F ₄ + 4.11 ⁷ F ₁
38	Γ ₁		4826	75.89 ⁷ F ₃ + 11.86 ⁷ F ₂ + 10.13 ⁷ F ₄
39	Γ ₂		4889	74.05 ⁷ F ₃ + 16.14 ⁷ F ₂ + 8.95 ⁷ F ₄
40	Γ ₂		4981	91.46 ⁷ F ₃ + 6.76 ⁷ F ₄ + 0.80 ⁷ F ₅
41	Γ ₂	⁷ F ₂	5296	71.96 ⁷ F ₂ + 24.73 ⁷ F ₃ + 2.15 ⁷ F ₄
42	Γ ₁	5028	5363	79.11 ⁷ F ₂ + 9.33 ⁷ F ₀ + 7.73 ⁷ F ₃
43	Γ ₂	⁷ F ₁	5559	91.29 ⁷ F ₂ + 4.10 ⁷ F ₁ + 1.58 ⁷ F ₃
44	Γ ₁	5481	5707	55.08 ⁷ F ₂ + 33.96 ⁷ F ₁ + 8.92 ⁷ F ₃
45	Γ ₁		5788	46.71 ⁷ F ₂ + 39.60 ⁷ F ₁ + 12.64 ⁷ F ₃
46	Γ ₁		5826	73.55 ⁷ F ₂ + 16.79 ⁷ F ₁ + 8.00 ⁷ F ₃
47	Γ ₂		6158	90.88 ⁷ F ₁ + 3.98 ⁷ F ₃ + 3.66 ⁷ F ₂
48	Γ ₂		6189	91.91 ⁷ F ₁ + 4.21 ⁷ F ₃ + 2.74 ⁷ F ₂

Table 31 (cont'd).
Predicted energy
levels for Tb³⁺ in
Ca₅(PO₄)₃F, C_s site.
B_{nm} from table 9.

Level	I. R.	[(S,L)] ^a	Energy (cm ⁻¹)	Free ion mixture (%)
49	Γ ₁	⁷ F ₀ 5703	6307	85.53 ⁷ F ₀ + 12.33 ⁷ F ₂ + 1.90 ⁷ F ₄
50	Γ ₁	⁵ D ₄	20834	99.87 ⁵ D ₄ + 0.07 ⁵ G ₆ + 0.02 ⁵ L ₁₀
51	Γ ₁	20542	20836	99.87 ⁵ D ₄ + 0.07 ⁵ G ₆ + 0.02 ⁵ G ₅
52	Γ ₂		20935	99.73 ⁵ D ₄ + 0.16 ⁵ G ₆ + 0.04 ⁵ G ₅
53	Γ ₁		20939	99.68 ⁵ D ₄ + 0.22 ⁵ G ₆ + 0.03 ⁵ G ₅
54	Γ ₂		20958	99.82 ⁵ D ₄ + 0.06 ⁵ G ₆ + 0.06 ⁵ D ₃
55	Γ ₂		20970	99.85 ⁵ D ₄ + 0.05 ⁵ G ₆ + 0.05 ⁵ D ₃
56	Γ ₁		21025	99.83 ⁵ D ₄ + 0.08 ⁵ G ₆ + 0.04 ⁵ D ₃
57	Γ ₁		21074	99.88 ⁵ D ₄ + 0.03 ⁵ G ₆ + 0.02 ⁵ L ₁₀
58	Γ ₂		21078	99.88 ⁵ D ₄ + 0.05 ⁵ G ₆ + 0.02 ⁵ L ₁₀
59	Γ ₁	⁵ G ₆	26498	94.72 ⁵ G ₆ + 2.60 ⁵ D ₃ + 1.27 ⁵ L ₁₀
60	Γ ₁	26424	26500	94.74 ⁵ G ₆ + 2.60 ⁵ D ₃ + 1.31 ⁵ L ₁₀
61	Γ ₂	⁵ D ₃	26580	69.67 ⁵ G ₆ + 29.04 ⁵ D ₃ + 0.49 ⁵ L ₁₀
62	Γ ₂	26336	26601	74.49 ⁵ G ₆ + 23.56 ⁵ D ₃ + 0.95 ⁵ L ₁₀
63	Γ ₁		26688	61.68 ⁵ D ₃ + 36.35 ⁵ G ₆ + 0.83 ⁵ G ₅
64	Γ ₁		26724	81.15 ⁵ D ₃ + 17.78 ⁵ G ₆ + 0.34 ⁵ G ₅
65	Γ ₁		26731	49.31 ⁵ G ₆ + 45.29 ⁵ D ₃ + 3.62 ⁵ L ₁₀
66	Γ ₂		26737	82.48 ⁵ D ₃ + 14.96 ⁵ G ₆ + 1.18 ⁵ G ₅
67	Γ ₂		26743	68.35 ⁵ D ₃ + 29.51 ⁵ G ₆ + 1.17 ⁵ L ₁₀
68	Γ ₁		26756	62.83 ⁵ D ₃ + 34.10 ⁵ G ₆ + 1.99 ⁵ L ₁₀
69	Γ ₂		26769	83.39 ⁵ D ₃ + 15.23 ⁵ G ₆ + 0.73 ⁵ G ₅
70	Γ ₂		26777	72.33 ⁵ D ₃ + 26.22 ⁵ G ₆ + 0.93 ⁵ L ₁₀
71	Γ ₁		26794	76.58 ⁵ G ₆ + 21.27 ⁵ D ₃ + 1.00 ⁵ L ₁₀
72	Γ ₂		26842	77.59 ⁵ G ₆ + 14.07 ⁵ D ₃ + 6.02 ⁵ L ₁₀
73	Γ ₂		26931	85.79 ⁵ G ₆ + 10.78 ⁵ D ₃ + 1.37 ⁵ G ₅
74	Γ ₁		27003	73.95 ⁵ G ₆ + 13.32 ⁵ L ₁₀ + 10.29 ⁵ D ₃
75	Γ ₁		27012	93.57 ⁵ G ₆ + 2.87 ⁵ D ₃ + 2.16 ⁵ L ₁₀
76	Γ ₂		27020	87.78 ⁵ G ₆ + 7.46 ⁵ L ₁₀ + 2.67 ⁵ D ₃
77	Γ ₁		27056	88.18 ⁵ G ₆ + 5.09 ⁵ D ₃ + 4.67 ⁵ L ₁₀
78	Γ ₂		27090	83.53 ⁵ G ₆ + 8.40 ⁵ D ₃ + 5.89 ⁵ L ₁₀
79	Γ ₂	⁵ L ₁₀	27142	81.76 ⁵ L ₁₀ + 17.33 ⁵ G ₆ + 0.45 ⁵ D ₃
80	Γ ₁	27146	27145	79.73 ⁵ L ₁₀ + 19.04 ⁵ G ₆ + 0.67 ⁵ D ₃
81	Γ ₁	⁵ G ₅	27224	98.05 ⁵ L ₁₀ + 1.39 ⁵ G ₆ + 0.45 ⁵ L ₉
82	Γ ₁	27795	27225	97.67 ⁵ L ₁₀ + 1.69 ⁵ G ₆ + 0.51 ⁵ L ₉
83	Γ ₂		27294	98.73 ⁵ L ₁₀ + 0.56 ⁵ G ₆ + 0.43 ⁵ L ₉
84	Γ ₂		27299	98.21 ⁵ L ₁₀ + 0.93 ⁵ G ₆ + 0.56 ⁵ L ₉
85	Γ ₁		27449	97.06 ⁵ L ₁₀ + 1.60 ⁵ L ₉ + 1.17 ⁵ G ₆
86	Γ ₁		27476	96.13 ⁵ L ₁₀ + 2.27 ⁵ L ₉ + 1.41 ⁵ G ₆
87	Γ ₂		27477	93.69 ⁵ L ₁₀ + 4.30 ⁵ L ₉ + 1.72 ⁵ G ₆
88	Γ ₁		27491	95.83 ⁵ L ₁₀ + 2.98 ⁵ L ₉ + 1.09 ⁵ G ₆
89	Γ ₂		27544	97.24 ⁵ L ₁₀ + 1.38 ⁵ L ₉ + 0.87 ⁵ G ₆
90	Γ ₂		27600	96.09 ⁵ L ₁₀ + 1.87 ⁵ G ₆ + 1.38 ⁵ L ₉
91	Γ ₁		27646	97.19 ⁵ L ₁₀ + 1.35 ⁵ L ₉ + 1.35 ⁵ G ₆
92	Γ ₁		27690	97.46 ⁵ L ₁₀ + 1.71 ⁵ L ₉ + 0.68 ⁵ G ₆
93	Γ ₂		27690	97.55 ⁵ L ₁₀ + 1.64 ⁵ L ₉ + 0.44 ⁵ G ₆
94	Γ ₂		27771	96.58 ⁵ L ₁₀ + 1.76 ⁵ G ₅ + 0.84 ⁵ G ₆
95	Γ ₁		27773	96.97 ⁵ L ₁₀ + 1.12 ⁵ G ₆ + 1.09 ⁵ G ₅
96	Γ ₂		27932	48.91 ⁵ G ₅ + 48.17 ⁵ L ₁₀ + 1.50 ⁵ G ₄

Table 31 (cont'd).
Predicted energy
levels for Tb^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
97	Γ_2		27939	$53.31 {}^5L_{10} + 44.33 {}^5G_5 + 1.21 {}^5G_4$
98	Γ_1		27977	$90.21 {}^5L_{10} + 8.83 {}^5G_5 + 0.51 {}^5L_9$
99	Γ_1		27981	$89.45 {}^5L_{10} + 9.64 {}^5G_5 + 0.46 {}^5L_9$
100	Γ_2		28036	$50.38 {}^5L_{10} + 44.99 {}^5G_5 + 2.55 {}^5G_4$
101	Γ_2		28039	$51.89 {}^5G_5 + 43.56 {}^5L_{10} + 2.94 {}^5G_4$
102	Γ_1		28145	$84.92 {}^5G_5 + 8.04 {}^5L_{10} + 3.92 {}^5G_4$
103	Γ_1		28161	$86.76 {}^5G_5 + 8.61 {}^5L_{10} + 2.84 {}^5D_2$
104	Γ_2		28182	$84.13 {}^5G_5 + 8.74 {}^5G_4 + 3.07 {}^5L_{10}$
105	Γ_1		28255	$87.10 {}^5G_5 + 9.53 {}^5G_4 + 1.30 {}^5L_{10}$
106	Γ_2		28259	$94.20 {}^5G_5 + 1.99 {}^5G_4 + 1.64 {}^5G_6$
107	Γ_1		28282	$85.85 {}^5G_5 + 9.41 {}^5G_4 + 1.81 {}^5D_2$
108	Γ_2		28349	$87.48 {}^5G_5 + 5.69 {}^5G_4 + 4.70 {}^5D_2$
109	Γ_2		28366	$90.89 {}^5G_5 + 4.61 {}^5D_2 + 2.09 {}^5G_4$
110	Γ_1		28377	$83.71 {}^5G_5 + 9.34 {}^5G_4 + 4.12 {}^5D_2$
111	Γ_2	5D_2	28490	$85.95 {}^5D_2 + 8.57 {}^5G_5 + 4.48 {}^5G_4$
112	Γ_1	28150	28505	$82.53 {}^5D_2 + 13.15 {}^5G_4 + 3.61 {}^5G_5$
113	Γ_2	5G_4	28562	$73.91 {}^5D_2 + 18.43 {}^5G_4 + 5.90 {}^5G_5$
114	Γ_1	28307	28595	$52.44 {}^5G_4 + 43.56 {}^5D_2 + 2.03 {}^5L_9$
115	Γ_1	5L_9	28624	$84.77 {}^5G_4 + 7.18 {}^5D_2 + 4.39 {}^5G_5$
116	Γ_2	28503	28640	$96.68 {}^5L_9 + 2.05 {}^5G_4 + 0.65 {}^5L_{10}$
117	Γ_2		28642	$96.27 {}^5L_9 + 2.17 {}^5G_4 + 0.62 {}^5L_{10}$
118	Γ_1		28657	$71.65 {}^5D_2 + 18.79 {}^5G_4 + 5.54 {}^5L_9$
119	Γ_1		28668	$35.09 {}^5L_9 + 31.45 {}^5G_4 + 22.96 {}^5D_2$
120	Γ_2		28677	$92.70 {}^5L_9 + 3.58 {}^5L_{10} + 1.33 {}^5G_5$
121	Γ_1		28681	$56.52 {}^5L_9 + 20.48 {}^5D_2 + 13.89 {}^5G_4$
122	Γ_1		28751	$92.33 {}^5L_9 + 3.56 {}^5G_4 + 2.37 {}^5D_2$
123	Γ_1		28761	$89.88 {}^5L_9 + 6.91 {}^5G_4 + 1.30 {}^5L_{10}$
124	Γ_2		28765	$90.06 {}^5G_4 + 4.95 {}^5G_5 + 4.56 {}^5L_9$
125	Γ_2		28797	$86.05 {}^5G_4 + 5.17 {}^5G_5 + 4.30 {}^5L_9$
126	Γ_1		28853	$80.07 {}^5G_4 + 11.03 {}^5D_2 + 6.59 {}^5L_9$
127	Γ_2		28860	$60.88 {}^5G_4 + 24.35 {}^5L_9 + 7.02 {}^5D_2$
128	Γ_1		28875	$75.75 {}^5G_4 + 13.01 {}^5D_2 + 5.53 {}^5G_5$
129	Γ_2		28879	$49.16 {}^5G_4 + 35.59 {}^5L_9 + 8.61 {}^5D_2$
130	Γ_1		28881	$66.18 {}^5G_4 + 15.63 {}^5L_9 + 9.85 {}^5D_2$
131	Γ_2		28911	$61.97 {}^5L_9 + 35.02 {}^5G_4 + 1.73 {}^5D_2$
132	Γ_2		28924	$81.13 {}^5L_9 + 14.83 {}^5G_4 + 1.58 {}^5D_2$
133	Γ_1		28966	$85.16 {}^5L_9 + 11.49 {}^5G_4 + 1.22 {}^5D_2$
134	Γ_2		28974	$95.37 {}^5L_9 + 2.71 {}^5G_4 + 1.41 {}^5L_{10}$
135	Γ_1		28991	$97.92 {}^5L_9 + 0.90 {}^5G_4 + 0.77 {}^5L_{10}$
136	Γ_1		29041	$98.17 {}^5L_9 + 0.71 {}^5L_{10} + 0.65 {}^5G_6$
137	Γ_2		29068	$98.60 {}^5L_9 + 0.81 {}^5G_6 + 0.32 {}^5L_{10}$
138	Γ_2		29141	$96.15 {}^5L_9 + 2.51 {}^5G_4 + 0.75 {}^5G_6$
139	Γ_1		29151	$95.69 {}^5L_9 + 2.98 {}^5G_4 + 0.90 {}^5G_6$
140	Γ_1		29249	$96.68 {}^5L_9 + 2.04 {}^5L_{10} + 0.99 {}^5G_4$
141	Γ_2		29249	$96.97 {}^5L_9 + 1.93 {}^5L_{10} + 0.76 {}^5G_4$
142	Γ_1		29255	$96.79 {}^5L_9 + 1.85 {}^5L_{10} + 0.92 {}^5G_4$
143	Γ_2		29257	$96.77 {}^5L_9 + 1.68 {}^5L_{10} + 1.06 {}^5G_4$

^aAqueous centroids (cm^{-1}).

Table 32. Predicted energy levels for Dy³⁺ in Ca₅(PO₄)₃F, C_s site. B_{nm} from table 9.

Level	[(S,L)] ^a	Energy (cm ⁻¹)	Free ion mixture (%)
1	⁶ H _{15/2} 40	0	99.72 ⁶ H _{15/2} + 0.12 ⁶ F _{11/2} + 0.11 ⁶ H _{13/2}
2		286	99.29 ⁶ H _{15/2} + 0.60 ⁶ H _{13/2} + 0.07 ⁶ F _{9/2}
3		461	99.37 ⁶ H _{15/2} + 0.31 ⁶ F _{11/2} + 0.26 ⁶ H _{13/2}
4		564	99.32 ⁶ H _{15/2} + 0.49 ⁶ H _{13/2} + 0.10 ⁶ F _{11/2}
5		722	99.49 ⁶ H _{15/2} + 0.37 ⁶ H _{13/2} + 0.06 ⁶ F _{11/2}
6		765	99.36 ⁶ H _{15/2} + 0.44 ⁶ H _{13/2} + 0.11 ⁶ F _{11/2}
7		883	99.38 ⁶ H _{15/2} + 0.28 ⁶ F _{11/2} + 0.21 ⁶ H _{13/2}
8		1016	99.56 ⁶ H _{15/2} + 0.23 ⁶ F _{11/2} + 0.10 ⁶ F _{9/2}
9	⁶ H _{13/2} 3506	3672	98.71 ⁶ H _{13/2} + 0.58 ⁶ H _{15/2} + 0.34 ⁶ H _{11/2}
10		3869	97.43 ⁶ H _{13/2} + 1.48 ⁶ H _{11/2} + 0.73 ⁶ H _{15/2}
11		4029	98.20 ⁶ H _{13/2} + 1.04 ⁶ H _{11/2} + 0.40 ⁶ H _{15/2}
12		4090	98.75 ⁶ H _{13/2} + 0.40 ⁶ H _{11/2} + 0.28 ⁶ H _{15/2}
13		4123	97.96 ⁶ H _{13/2} + 1.00 ⁶ H _{11/2} + 0.42 ⁶ F _{11/2}
14		4194	98.11 ⁶ H _{13/2} + 0.94 ⁶ H _{11/2} + 0.25 ⁶ H _{15/2}
15		4361	98.76 ⁶ H _{13/2} + 0.38 ⁶ H _{11/2} + 0.25 ⁶ F _{11/2}
16	⁶ H _{11/2} 5833	6117	97.22 ⁶ H _{11/2} + 1.63 ⁶ H _{13/2} + 0.45 ⁶ H _{9/2}
17		6217	95.86 ⁶ H _{11/2} + 1.61 ⁶ H _{9/2} + 1.50 ⁶ H _{13/2}
18		6337	96.90 ⁶ H _{11/2} + 0.86 ⁶ H _{9/2} + 0.76 ⁶ F _{9/2}
19		6436	96.19 ⁶ H _{11/2} + 1.52 ⁶ H _{9/2} + 0.80 ⁶ F _{9/2}
20		6534	96.72 ⁶ H _{11/2} + 1.07 ⁶ H _{9/2} + 0.87 ⁶ F _{11/2}
21		6610	97.52 ⁶ H _{11/2} + 0.90 ⁶ F _{11/2} + 0.85 ⁶ H _{13/2}
22	⁶ H _{9/2} 7692	7980	81.83 ⁶ H _{9/2} + 13.74 ⁶ F _{11/2} + 2.46 ⁶ H _{11/2}
23		8027	69.92 ⁶ H _{9/2} + 24.75 ⁶ F _{11/2} + 2.61 ⁶ H _{7/2}
24		8128	55.99 ⁶ F _{11/2} + 40.68 ⁶ H _{9/2} + 0.87 ⁶ H _{7/2}
25		8196	60.12 ⁶ F _{11/2} + 37.36 ⁶ H _{9/2} + 0.87 ⁶ F _{9/2}
26		8250	61.22 ⁶ F _{11/2} + 35.67 ⁶ H _{9/2} + 1.10 ⁶ F _{9/2}
27		8273	49.07 ⁶ F _{11/2} + 47.09 ⁶ H _{9/2} + 1.04 ⁶ H _{7/2}
28		8321	59.06 ⁶ F _{11/2} + 38.73 ⁶ H _{9/2} + 0.61 ⁶ F _{9/2}
29		8366	54.64 ⁶ F _{11/2} + 42.78 ⁶ H _{9/2} + 1.18 ⁶ F _{9/2}
30	⁶ F _{11/2} 7730	8424	64.59 ⁶ F _{11/2} + 33.38 ⁶ H _{9/2} + 0.58 ⁶ H _{7/2}
31		8541	84.55 ⁶ F _{11/2} + 12.91 ⁶ H _{9/2} + 0.93 ⁶ H _{11/2}
32		8625	63.34 ⁶ F _{11/2} + 33.26 ⁶ H _{9/2} + 1.31 ⁶ H _{7/2}
33		9401	62.72 ⁶ H _{7/2} + 30.69 ⁶ F _{9/2} + 4.43 ⁶ H _{9/2}
34		9469	73.28 ⁶ H _{7/2} + 18.69 ⁶ F _{9/2} + 4.98 ⁶ H _{5/2}
35		9606	59.63 ⁶ F _{9/2} + 37.47 ⁶ H _{7/2} + 0.87 ⁶ H _{9/2}
36		9650	55.16 ⁶ F _{9/2} + 40.01 ⁶ H _{7/2} + 1.42 ⁶ H _{9/2}
37		9689	82.18 ⁶ F _{9/2} + 14.41 ⁶ H _{7/2} + 1.34 ⁶ H _{9/2}
38	⁶ H _{7/2} 9087	9741	88.19 ⁶ F _{9/2} + 9.44 ⁶ H _{7/2} + 0.90 ⁶ H _{9/2}
39		9819	66.88 ⁶ F _{9/2} + 27.38 ⁶ H _{7/2} + 2.60 ⁶ H _{5/2}
40		9833	50.40 ⁶ F _{9/2} + 42.72 ⁶ H _{7/2} + 3.61 ⁶ H _{5/2}
41		9964	59.75 ⁶ H _{7/2} + 31.76 ⁶ F _{9/2} + 3.74 ⁶ H _{5/2}
42		10546	83.63 ⁶ H _{5/2} + 11.77 ⁶ H _{7/2} + 2.11 ⁶ F _{9/2}
43		10764	91.74 ⁶ H _{5/2} + 2.73 ⁶ H _{7/2} + 2.23 ⁶ F _{7/2}
44		10947	87.71 ⁶ H _{5/2} + 8.61 ⁶ F _{7/2} + 1.10 ⁶ H _{7/2}
45		11621	95.78 ⁶ F _{7/2} + 2.41 ⁶ H _{5/2} + 0.67 ⁶ H _{7/2}
46	⁶ F _{7/2} 11025	11649	92.59 ⁶ F _{7/2} + 4.84 ⁶ H _{5/2} + 1.14 ⁶ H _{7/2}
47		11694	97.66 ⁶ F _{7/2} + 0.85 ⁶ H _{7/2} + 0.48 ⁶ H _{9/2}
48		11736	93.35 ⁶ F _{7/2} + 3.90 ⁶ H _{5/2} + 1.38 ⁶ H _{7/2}

Table 32 (cont'd).
Predicted energy
levels for Dy^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
49	$6F_{5/2}$	13008	$96.41\ 6F_{5/2} + 1.23\ 6H_{5/2} + 1.04\ 6F_{3/2}$
50	12432	13052	$97.37\ 6F_{5/2} + 1.06\ 6F_{3/2} + 0.67\ 6H_{7/2}$
51		13122	$97.58\ 6F_{5/2} + 1.24\ 6H_{5/2} + 0.38\ 6F_{7/2}$
52	$6F_{3/2}$	13825	$96.61\ 6F_{3/2} + 1.79\ 6F_{1/2} + 0.58\ 6H_{5/2}$
53	13212	13865	$96.27\ 6F_{3/2} + 2.11\ 6F_{5/2} + 0.69\ 6H_{5/2}$
54	$6F_{1/2}$	14401	$96.62\ 6F_{1/2} + 2.01\ 6F_{3/2} + 0.54\ 6H_{5/2}$
	13760		
55	$4F_{9/2}$	21456	$97.42\ 4F_{9/2} + 2.02\ 4I_{15/2} + 0.55\ 4G_{11/2}$
56	21144	21560	$96.33\ 4F_{9/2} + 2.68\ 4I_{15/2} + 0.99\ 4G_{11/2}$
57		21633	$97.24\ 4F_{9/2} + 1.73\ 4I_{15/2} + 1.03\ 4G_{11/2}$
58		21774	$92.89\ 4F_{9/2} + 5.53\ 4I_{15/2} + 1.57\ 4G_{11/2}$
59		21865	$93.57\ 4F_{9/2} + 5.38\ 4I_{15/2} + 1.05\ 4G_{11/2}$
60	$4I_{15/2}$	22457	$98.87\ 4I_{15/2} + 0.94\ 4G_{11/2} + 0.19\ 4F_{9/2}$
61	22293	22708	$93.35\ 4I_{15/2} + 6.10\ 4F_{9/2} + 0.55\ 4G_{11/2}$
62		22746	$97.43\ 4I_{15/2} + 1.66\ 4G_{11/2} + 0.90\ 4F_{9/2}$
63		22889	$95.14\ 4I_{15/2} + 3.39\ 4F_{9/2} + 1.46\ 4G_{11/2}$
64		22957	$96.06\ 4I_{15/2} + 3.08\ 4G_{11/2} + 0.86\ 4F_{9/2}$
65		23003	$96.88\ 4I_{15/2} + 2.06\ 4G_{11/2} + 1.05\ 4F_{9/2}$
66		23045	$94.90\ 4I_{15/2} + 2.57\ 4F_{9/2} + 2.53\ 4G_{11/2}$
67		23219	$95.57\ 4I_{15/2} + 2.30\ 4G_{11/2} + 2.13\ 4F_{9/2}$
68	$4G_{11/2}$	23669	$96.58\ 4G_{11/2} + 3.17\ 4I_{15/2} + 0.25\ 4F_{9/2}$
69	23321	23788	$95.24\ 4G_{11/2} + 3.76\ 4I_{15/2} + 1.00\ 4F_{9/2}$
70		23944	$95.57\ 4G_{11/2} + 2.58\ 4I_{15/2} + 1.85\ 4F_{9/2}$
71		24034	$97.08\ 4G_{11/2} + 1.57\ 4I_{15/2} + 1.35\ 4F_{9/2}$
72		24088	$97.85\ 4G_{11/2} + 1.58\ 4I_{15/2} + 0.56\ 4F_{9/2}$
73		24120	$97.90\ 4G_{11/2} + 1.78\ 4I_{15/2} + 0.32\ 4F_{9/2}$

^aAqueous centroids (cm^{-1}).

Table 33. Predicted
energy levels for Ho^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$5I_8$	0	$99.93\ 5I_8 + 0.04\ 5I_7 + 0.01\ 5G_6$
2	Γ_1	80	2	$99.93\ 5I_8 + 0.04\ 5I_7 + 0.01\ 5G_6$
3	Γ_2		94	$99.89\ 5I_8 + 0.06\ 5I_7 + 0.02\ 5F_5$
4	Γ_2		105	$99.89\ 5I_8 + 0.07\ 5I_7 + 0.02\ 5F_5$
5	Γ_1		163	$99.91\ 5I_8 + 0.05\ 5I_7 + 0.02\ 5G_6$
6	Γ_2		178	$99.93\ 5I_8 + 0.03\ 5I_7 + 0.02\ 5G_6$
7	Γ_1		238	$99.82\ 5I_8 + 0.13\ 5I_7 + 0.02\ 5F_5$
8	Γ_1		290	$99.91\ 5I_8 + 0.06\ 5I_7 + 0.01\ 5G_6$
9	Γ_2		316	$99.90\ 5I_8 + 0.04\ 5I_7 + 0.03\ 5G_6$
10	Γ_1		343	$99.93\ 5I_8 + 0.03\ 5I_7 + 0.02\ 5G_6$
11	Γ_2		395	$99.89\ 5I_8 + 0.06\ 5I_7 + 0.03\ 5G_6$
12	Γ_2		403	$99.90\ 5I_8 + 0.05\ 5I_7 + 0.04\ 5G_6$
13	Γ_1		413	$99.89\ 5I_8 + 0.05\ 5I_7 + 0.04\ 5G_6$
14	Γ_2		428	$99.85\ 5I_8 + 0.11\ 5I_7 + 0.02\ 5G_6$
15	Γ_1		467	$99.88\ 5I_8 + 0.06\ 5I_7 + 0.04\ 5G_6$
16	Γ_1		553	$99.85\ 5I_8 + 0.06\ 5I_7 + 0.04\ 5G_6$
17	Γ_2		556	$99.86\ 5I_8 + 0.06\ 5I_7 + 0.05\ 5G_6$

Table 33 (cont'd).
Predicted energy
levels for Ho^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
18	Γ_2	5I_7	5116	$99.81\ ^5I_7 + 0.08\ ^5I_6 + 0.05\ ^5I_8$
19	Γ_1	5116	5116	$99.81\ ^5I_7 + 0.08\ ^5I_6 + 0.06\ ^5I_8$
20	Γ_2		5229	$99.72\ ^5I_7 + 0.13\ ^5I_6 + 0.10\ ^5I_8$
21	Γ_1		5230	$99.68\ ^5I_7 + 0.13\ ^5I_8 + 0.13\ ^5I_6$
22	Γ_2		5282	$99.84\ ^5I_7 + 0.06\ ^5I_8 + 0.05\ ^5I_6$
23	Γ_1		5283	$99.84\ ^5I_7 + 0.07\ ^5I_8 + 0.03\ ^5I_6$
24	Γ_2		5332	$99.68\ ^5I_7 + 0.17\ ^5I_6 + 0.09\ ^5I_8$
25	Γ_2		5335	$99.64\ ^5I_7 + 0.16\ ^5I_6 + 0.11\ ^5I_8$
26	Γ_1		5392	$99.69\ ^5I_7 + 0.20\ ^5I_6 + 0.04\ ^5I_8$
27	Γ_2		5398	$99.79\ ^5I_7 + 0.11\ ^5I_6 + 0.04\ ^5I_8$
28	Γ_1		5403	$99.68\ ^5I_7 + 0.18\ ^5I_6 + 0.06\ ^5I_8$
29	Γ_1		5407	$99.85\ ^5I_7 + 0.05\ ^5I_8 + 0.03\ ^5F_5$
30	Γ_2		5424	$99.77\ ^5I_7 + 0.11\ ^5I_6 + 0.04\ ^5F_5$
31	Γ_1		5496	$99.68\ ^5I_7 + 0.14\ ^5I_6 + 0.06\ ^5I_8$
32	Γ_2		5497	$99.73\ ^5I_7 + 0.11\ ^5I_6 + 0.05\ ^5I_8$
33	Γ_1	5I_6	8635	$99.62\ ^5I_6 + 0.14\ ^5I_7 + 0.14\ ^5I_5$
34	Γ_1	8614	8635	$99.59\ ^5I_6 + 0.16\ ^5I_7 + 0.15\ ^5I_5$
35	Γ_2		8753	$99.36\ ^5I_6 + 0.29\ ^5I_7 + 0.25\ ^5I_5$
36	Γ_2		8760	$99.34\ ^5I_6 + 0.32\ ^5I_5 + 0.23\ ^5I_7$
37	Γ_1		8806	$99.72\ ^5I_6 + 0.12\ ^5I_7 + 0.07\ ^5I_5$
38	Γ_2		8813	$99.68\ ^5I_6 + 0.17\ ^5I_5 + 0.09\ ^5I_7$
39	Γ_1		8847	$99.36\ ^5I_6 + 0.36\ ^5I_5 + 0.16\ ^5I_7$
40	Γ_1		8854	$99.43\ ^5I_6 + 0.35\ ^5I_5 + 0.10\ ^5I_7$
41	Γ_2		8881	$99.47\ ^5I_6 + 0.38\ ^5I_5 + 0.04\ ^5F_5$
42	Γ_1		8916	$99.47\ ^5I_6 + 0.40\ ^5I_5 + 0.04\ ^5I_7$
43	Γ_2		8919	$99.62\ ^5I_6 + 0.21\ ^5I_5 + 0.05\ ^5I_7$
44	Γ_2		8966	$99.31\ ^5I_6 + 0.40\ ^5I_5 + 0.15\ ^5I_7$
45	Γ_1		8972	$99.52\ ^5I_6 + 0.21\ ^5I_5 + 0.13\ ^5I_7$
46	Γ_2	5I_5	11211	$99.03\ ^5I_5 + 0.46\ ^5I_6 + 0.37\ ^5I_4$
47	Γ_2	11164	11216	$99.31\ ^5I_5 + 0.38\ ^5I_6 + 0.18\ ^5I_4$
48	Γ_1		11342	$98.81\ ^5I_5 + 0.55\ ^5I_6 + 0.53\ ^5I_4$
49	Γ_1		11349	$98.97\ ^5I_5 + 0.53\ ^5I_6 + 0.44\ ^5I_4$
50	Γ_1		11375	$99.20\ ^5I_5 + 0.42\ ^5I_4 + 0.31\ ^5I_6$
51	Γ_2		11382	$99.47\ ^5I_5 + 0.30\ ^5I_6 + 0.16\ ^5I_4$
52	Γ_2		11414	$99.34\ ^5I_5 + 0.45\ ^5I_4 + 0.10\ ^5I_6$
53	Γ_2		11438	$99.33\ ^5I_5 + 0.38\ ^5I_4 + 0.16\ ^5I_6$
54	Γ_1		11454	$99.15\ ^5I_5 + 0.67\ ^5I_4 + 0.06\ ^5I_6$
55	Γ_1		11504	$99.00\ ^5I_5 + 0.63\ ^5I_4 + 0.25\ ^5I_6$
56	Γ_2		11506	$98.84\ ^5I_5 + 0.71\ ^5I_4 + 0.33\ ^5I_6$
57	Γ_1	5I_4	13205	$99.21\ ^5I_4 + 0.63\ ^5I_5 + 0.06\ ^5I_6$
58	Γ_1	13219	13241	$98.58\ ^5I_4 + 1.29\ ^5I_5 + 0.03\ ^5F_2$
59	Γ_2		13360	$99.47\ ^5I_4 + 0.39\ ^5I_5 + 0.04\ ^5F_3$
60	Γ_1		13425	$99.47\ ^5I_4 + 0.38\ ^5I_5 + 0.06\ ^5I_6$
61	Γ_2		13431	$99.09\ ^5I_4 + 0.71\ ^5I_5 + 0.08\ ^5F_2$
62	Γ_2		13504	$99.17\ ^5I_4 + 0.69\ ^5I_5 + 0.05\ ^5I_6$
63	Γ_1		13527	$99.72\ ^5I_4 + 0.13\ ^5I_5 + 0.03\ ^5I_6$
64	Γ_2		13655	$99.37\ ^5I_4 + 0.49\ ^5I_5 + 0.03\ ^5F_1$
65	Γ_1		13679	$99.58\ ^5I_4 + 0.27\ ^5I_5 + 0.05\ ^5I_6$

Table 33 (cont'd).
Predicted energy
levels for Ho^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
66	Γ_1	5F_5	15552	$99.51\ ^5F_5 + 0.19\ ^5F_4 + 0.11\ ^5G_6$
67	Γ_2	15519	15555	$99.54\ ^5F_5 + 0.14\ ^5F_4 + 0.10\ ^5G_6$
68	Γ_2		15608	$99.34\ ^5F_5 + 0.32\ ^5G_6 + 0.16\ ^5F_4$
69	Γ_1		15634	$99.51\ ^5F_5 + 0.28\ ^5G_6 + 0.06\ ^5F_4$
70	Γ_2		15637	$99.05\ ^5F_5 + 0.38\ ^5G_6 + 0.36\ ^5F_4$
71	Γ_1		15667	$99.17\ ^5F_5 + 0.40\ ^5G_6 + 0.26\ ^5F_4$
72	Γ_2		15716	$99.18\ ^5F_5 + 0.44\ ^5F_4 + 0.18\ ^5G_6$
73	Γ_1		15863	$99.37\ ^5F_5 + 0.24\ ^5F_4 + 0.20\ ^5G_6$
74	Γ_1		15874	$99.36\ ^5F_5 + 0.29\ ^5F_4 + 0.18\ ^5G_6$
75	Γ_2		15910	$99.49\ ^5F_5 + 0.27\ ^5G_6 + 0.05\ ^3G_5$
76	Γ_2		15918	$99.50\ ^5F_5 + 0.24\ ^5G_6 + 0.05\ ^3G_5$
77	Γ_2	5S_2	18527	$95.89\ ^5S_2 + 3.45\ ^5F_4 + 0.51\ ^5G_6$
78	Γ_1	18353	18540	$87.19\ ^5S_2 + 12.48\ ^5F_4 + 0.17\ ^5G_6$
79	Γ_1		18558	$97.94\ ^5S_2 + 1.56\ ^5F_4 + 0.28\ ^5G_6$
80	Γ_2		18564	$94.07\ ^5S_2 + 5.49\ ^5F_4 + 0.19\ ^5G_6$
81	Γ_1		18568	$96.66\ ^5S_2 + 2.64\ ^5F_4 + 0.61\ ^5G_6$
82	Γ_2	5F_4	18705	$95.74\ ^5F_4 + 3.33\ ^5S_2 + 0.35\ ^5F_3$
83	Γ_1	18612	18732	$87.29\ ^5F_4 + 11.75\ ^5S_2 + 0.34\ ^5F_2$
84	Γ_1		18750	$95.91\ ^5F_4 + 2.95\ ^5S_2 + 0.34\ ^5G_6$
85	Γ_2		18784	$96.11\ ^5F_4 + 3.02\ ^5S_2 + 0.23\ ^5F_2$
86	Γ_1		18831	$98.44\ ^5F_4 + 0.55\ ^5G_6 + 0.41\ ^5F_3$
87	Γ_2		18838	$95.71\ ^5F_4 + 2.53\ ^5S_2 + 0.60\ ^5G_6$
88	Γ_2		18874	$98.35\ ^5F_4 + 0.54\ ^5G_6 + 0.48\ ^5F_5$
89	Γ_1		18967	$97.91\ ^5F_4 + 0.96\ ^5S_2 + 0.25\ ^5F_3$
90	Γ_1		18973	$97.84\ ^5F_4 + 1.05\ ^5S_2 + 0.28\ ^5F_3$
91	Γ_2	3F_3	20706	$98.57\ ^5F_3 + 0.51\ ^5F_2 + 0.28\ ^3G_5$
92	Γ_1	20672	20786	$96.24\ ^5F_3 + 1.90\ ^5F_2 + 0.52\ ^5F_1$
93	Γ_1		20821	$95.22\ ^5F_3 + 2.77\ ^5F_2 + 0.81\ ^5G_6$
94	Γ_1		20897	$93.99\ ^5F_3 + 4.31\ ^5F_2 + 0.68\ ^5G_6$
95	Γ_2		20899	$92.78\ ^5F_3 + 5.42\ ^5F_2 + 0.77\ ^5G_6$
96	Γ_2		21007	$93.86\ ^5F_3 + 4.53\ ^5F_2 + 0.63\ ^5G_6$
97	Γ_2		21025	$96.75\ ^5F_3 + 1.64\ ^5F_2 + 0.47\ ^5G_6$
98	Γ_2	5F_2	21253	$89.00\ ^5F_2 + 9.37\ ^5F_3 + 1.03\ ^5F_1$
99	Γ_1	21130	21327	$98.47\ ^5F_2 + 0.39\ ^3K_8 + 0.38\ ^5F_4$
100	Γ_1	3K_8	21381	$92.21\ ^5F_2 + 5.35\ ^5F_3 + 1.13\ ^3K_8$
101	Γ_2	21307	21382	$93.79\ ^5F_2 + 2.65\ ^5F_3 + 1.14\ ^5F_1$
102	Γ_2		21427	$99.62\ ^3K_8 + 0.21\ ^5G_6 + 0.11\ ^5F_2$
103	Γ_1		21428	$99.23\ ^3K_8 + 0.49\ ^5F_2 + 0.22\ ^5G_6$
104	Γ_1		21461	$99.20\ ^3K_8 + 0.68\ ^5F_2 + 0.06\ ^5G_6$
105	Γ_1		21478	$86.72\ ^3K_8 + 12.44\ ^5F_2 + 0.50\ ^5F_3$
106	Γ_2		21479	$99.12\ ^3K_8 + 0.69\ ^5F_2 + 0.10\ ^5G_6$
107	Γ_2		21483	$99.88\ ^3K_8 + 0.07\ ^5G_6 + 0.03\ ^5F_2$
108	Γ_2		21485	$99.68\ ^3K_8 + 0.27\ ^5G_6 + 0.03\ ^5F_2$
109	Γ_1		21490	$82.04\ ^5F_2 + 14.10\ ^3K_8 + 3.02\ ^5F_3$
110	Γ_1		21510	$99.76\ ^3K_8 + 0.12\ ^5G_6 + 0.09\ ^5F_2$
111	Γ_2		21519	$99.77\ ^3K_8 + 0.19\ ^5G_6 + 0.01\ ^3G_5$
112	Γ_1		21530	$98.57\ ^3K_8 + 1.03\ ^5F_2 + 0.33\ ^5G_6$
113	Γ_1		21547	$99.79\ ^3K_8 + 0.11\ ^5G_6 + 0.07\ ^5F_2$
114	Γ_2		21577	$99.40\ ^3K_8 + 0.54\ ^5G_6 + 0.04\ ^5F_3$
115	Γ_1		21583	$99.56\ ^3K_8 + 0.39\ ^5G_6 + 0.03\ ^5F_3$

Table 33 (cont'd).
Predicted energy
levels for Ho^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
116	Γ_2		21602	$99.77 {}^3\text{K}_8 + 0.19 {}^5\text{G}_6 + 0.01 {}^5\text{F}_3$
117	Γ_2		21606	$99.76 {}^3\text{K}_8 + 0.20 {}^5\text{G}_6 + 0.01 {}^3\text{G}_5$
118	Γ_1		21640	$99.36 {}^3\text{K}_8 + 0.56 {}^5\text{G}_6 + 0.04 {}^5\text{F}_2$
119	Γ_1		21641	$99.48 {}^3\text{K}_8 + 0.43 {}^5\text{G}_6 + 0.08 {}^5\text{F}_2$
120	Γ_1	${}^5\text{G}_6$	22141	$97.52 {}^5\text{G}_6 + 0.59 {}^3\text{K}_8 + 0.52 {}^5\text{F}_4$
121	Γ_2	22094	22154	$97.99 {}^5\text{G}_6 + 0.50 {}^5\text{F}_4 + 0.40 {}^3\text{G}_5$
122	Γ_1	${}^5\text{F}_1$	22160	$97.76 {}^5\text{G}_6 + 0.57 {}^3\text{K}_8 + 0.37 {}^5\text{F}_2$
123	Γ_2	22375	22170	$97.53 {}^5\text{G}_6 + 0.64 {}^3\text{G}_5 + 0.61 {}^5\text{F}_1$
124	Γ_2		22264	$97.21 {}^5\text{G}_6 + 0.81 {}^5\text{F}_3 + 0.59 {}^3\text{G}_5$
125	Γ_1		22279	$97.05 {}^5\text{G}_6 + 0.88 {}^3\text{G}_5 + 0.70 {}^5\text{F}_3$
126	Γ_1		22330	$97.02 {}^5\text{G}_6 + 0.86 {}^3\text{G}_5 + 0.62 {}^5\text{F}_3$
127	Γ_2		22426	$98.03 {}^5\text{G}_6 + 0.42 {}^3\text{G}_5 + 0.39 {}^5\text{F}_5$
128	Γ_2		22478	$97.65 {}^5\text{G}_6 + 0.41 {}^5\text{F}_5 + 0.40 {}^5\text{F}_1$
129	Γ_1		22480	$57.93 {}^5\text{F}_1 + 39.88 {}^5\text{G}_6 + 1.09 {}^3\text{G}_5$
130	Γ_1		22512	$90.39 {}^5\text{G}_6 + 7.94 {}^5\text{F}_1 + 0.77 {}^3\text{G}_5$
131	Γ_1		22545	$71.57 {}^5\text{G}_6 + 27.04 {}^5\text{F}_1 + 0.68 {}^3\text{G}_5$
132	Γ_2		22554	$96.83 {}^5\text{G}_6 + 1.72 {}^5\text{F}_1 + 0.71 {}^3\text{G}_5$
133	Γ_1		22557	$94.25 {}^5\text{G}_6 + 4.49 {}^5\text{F}_1 + 0.27 {}^5\text{F}_2$
134	Γ_2		22673	$95.73 {}^5\text{F}_1 + 1.67 {}^5\text{G}_6 + 1.59 {}^5\text{F}_2$
135	Γ_2		22723	$97.27 {}^5\text{F}_1 + 1.19 {}^5\text{G}_6 + 0.71 {}^5\text{F}_2$
136	Γ_1	${}^3\text{G}_5$	24018	$98.73 {}^3\text{G}_5 + 0.45 {}^5\text{F}_3 + 0.29 {}^5\text{G}_6$
137	Γ_2	23887	24023	$98.99 {}^3\text{G}_5 + 0.34 {}^5\text{F}_3 + 0.34 {}^5\text{F}_2$
138	Γ_1		24079	$98.83 {}^3\text{G}_5 + 0.55 {}^5\text{G}_6 + 0.30 {}^5\text{F}_3$
139	Γ_2		24088	$99.19 {}^3\text{G}_5 + 0.30 {}^5\text{G}_6 + 0.26 {}^5\text{F}_3$
140	Γ_2		24103	$98.31 {}^3\text{G}_5 + 0.99 {}^5\text{G}_6 + 0.21 {}^5\text{F}_3$
141	Γ_1		24163	$99.00 {}^3\text{G}_5 + 0.69 {}^5\text{G}_6 + 0.11 {}^5\text{F}_4$
142	Γ_2		24177	$98.31 {}^3\text{G}_5 + 1.32 {}^5\text{G}_6 + 0.23 {}^5\text{F}_3$
143	Γ_1		24204	$97.87 {}^3\text{G}_5 + 1.42 {}^5\text{G}_6 + 0.34 {}^5\text{F}_2$
144	Γ_1		24212	$97.50 {}^3\text{G}_5 + 1.83 {}^5\text{G}_6 + 0.26 {}^5\text{F}_2$
145	Γ_2		24293	$99.42 {}^3\text{G}_5 + 0.26 {}^5\text{G}_6 + 0.11 {}^5\text{F}_5$
146	Γ_2		24296	$99.27 {}^3\text{G}_5 + 0.39 {}^5\text{G}_6 + 0.11 {}^5\text{F}_5$

^aAqueous centroids (cm^{-1}).

Table 34. Predicted
energy levels for
 Tm^{3+} in $\text{Ca}_5(\text{PO}_4)_3\text{F}$,
 C_s site. B_{nm} from table
9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	${}^3\text{H}_6$	0	$99.61 {}^3\text{H}_6 + 0.33 {}^3\text{F}_4 + 0.02 {}^3\text{H}_4$
2	Γ_2	202	9	$99.65 {}^3\text{H}_6 + 0.29 {}^3\text{F}_4 + 0.02 {}^3\text{F}_3$
3	Γ_2		143	$99.49 {}^3\text{H}_6 + 0.45 {}^3\text{F}_4 + 0.02 {}^3\text{H}_4$
4	Γ_1		145	$99.63 {}^3\text{H}_6 + 0.29 {}^3\text{F}_4 + 0.03 {}^3\text{H}_5$
5	Γ_2		292	$99.89 {}^3\text{H}_6 + 0.06 {}^3\text{H}_5 + 0.04 {}^3\text{F}_4$
6	Γ_1		373	$99.77 {}^3\text{H}_6 + 0.16 {}^3\text{F}_4 + 0.05 {}^3\text{H}_5$
7	Γ_1		406	$99.83 {}^3\text{H}_6 + 0.09 {}^3\text{F}_4 + 0.06 {}^3\text{H}_5$
8	Γ_2		513	$99.72 {}^3\text{H}_6 + 0.25 {}^3\text{F}_4 + 0.02 {}^3\text{H}_4$
9	Γ_1		534	$99.51 {}^3\text{H}_6 + 0.43 {}^3\text{F}_4 + 0.03 {}^3\text{H}_4$
10	Γ_2		691	$99.86 {}^3\text{H}_6 + 0.07 {}^3\text{H}_5 + 0.05 {}^3\text{F}_4$
11	Γ_2		726	$99.80 {}^3\text{H}_6 + 0.11 {}^3\text{F}_4 + 0.06 {}^3\text{H}_5$
12	Γ_1		1090	$99.71 {}^3\text{H}_6 + 0.24 {}^3\text{F}_4 + 0.03 {}^3\text{H}_5$
13	Γ_1		1092	$99.72 {}^3\text{H}_6 + 0.23 {}^3\text{F}_4 + 0.03 {}^3\text{H}_5$

Table 34 (cont'd).
Predicted energy
levels for Tm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S, L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
14	Γ_1	3F_4	5805	$99.45\ ^3F_4 + 0.28\ ^3H_6 + 0.12\ ^3H_5$
15	Γ_2	5812	5867	$99.23\ ^3F_4 + 0.34\ ^3H_6 + 0.32\ ^3H_5$
16	Γ_1		5892	$99.18\ ^3F_4 + 0.44\ ^3H_5 + 0.28\ ^3H_6$
17	Γ_2		5994	$98.97\ ^3F_4 + 0.85\ ^3H_5 + 0.16\ ^3H_6$
18	Γ_2		6096	$99.59\ ^3F_4 + 0.23\ ^3H_5 + 0.10\ ^3H_6$
19	Γ_1		6244	$98.83\ ^3F_4 + 0.69\ ^3H_5 + 0.34\ ^3H_6$
20	Γ_1		6263	$99.42\ ^3F_4 + 0.28\ ^3H_6 + 0.16\ ^3H_5$
21	Γ_1		6298	$98.75\ ^3F_4 + 0.63\ ^3H_6 + 0.51\ ^3H_5$
22	Γ_2		6338	$98.84\ ^3F_4 + 0.59\ ^3H_6 + 0.43\ ^3H_5$
23	Γ_2	3H_5	8258	$98.76\ ^3H_5 + 0.77\ ^3F_4 + 0.18\ ^3H_4$
24	Γ_1	8390	8264	$99.09\ ^3H_5 + 0.50\ ^3F_4 + 0.25\ ^3F_3$
25	Γ_1		8404	$98.68\ ^3H_5 + 0.74\ ^3F_4 + 0.34\ ^3H_4$
26	Γ_2		8458	$99.33\ ^3H_5 + 0.42\ ^3F_3 + 0.13\ ^3H_4$
27	Γ_2		8547	$99.38\ ^3H_5 + 0.28\ ^3H_4 + 0.24\ ^3F_4$
28	Γ_2		8682	$99.42\ ^3H_5 + 0.26\ ^3F_4 + 0.25\ ^3F_3$
29	Γ_1		8685	$99.14\ ^3H_5 + 0.42\ ^3F_4 + 0.32\ ^3F_3$
30	Γ_1		8781	$99.40\ ^3H_5 + 0.19\ ^3H_4 + 0.15\ ^3F_4$
31	Γ_1		8796	$99.52\ ^3H_5 + 0.16\ ^3H_4 + 0.13\ ^3F_4$
32	Γ_2		9186	$99.34\ ^3H_5 + 0.24\ ^3F_4 + 0.24\ ^3H_4$
33	Γ_2		9189	$99.30\ ^3H_5 + 0.26\ ^3F_4 + 0.22\ ^3H_4$
34	Γ_2	3H_4	12685	$97.03\ ^3H_4 + 2.49\ ^3F_3 + 0.24\ ^3F_2$
35	Γ_1	12720	12751	$97.81\ ^3H_4 + 1.65\ ^3F_3 + 0.43\ ^3F_2$
36	Γ_1		12758	$98.02\ ^3H_4 + 1.42\ ^3F_2 + 0.20\ ^3F_3$
37	Γ_2		12911	$97.31\ ^3H_4 + 1.94\ ^3F_2 + 0.36\ ^3F_3$
38	Γ_1		12990	$98.73\ ^3H_4 + 0.57\ ^3F_2 + 0.39\ ^3F_3$
39	Γ_2		12993	$99.39\ ^3H_4 + 0.38\ ^3H_5 + 0.12\ ^3F_3$
40	Γ_1		13081	$98.88\ ^3H_4 + 0.51\ ^3F_3 + 0.32\ ^3H_5$
41	Γ_1		13283	$97.43\ ^3H_4 + 1.91\ ^3F_3 + 0.27\ ^3F_2$
42	Γ_2		13309	$96.97\ ^3H_4 + 2.38\ ^3F_3 + 0.31\ ^3F_2$
43	Γ_2	3F_3	14677	$99.03\ ^3F_3 + 0.66\ ^3H_4 + 0.22\ ^3H_5$
44	Γ_2	14510	14719	$97.09\ ^3F_3 + 1.54\ ^3H_4 + 1.15\ ^3F_2$
45	Γ_1		14794	$95.52\ ^3F_3 + 2.13\ ^3H_4 + 2.01\ ^3F_2$
46	Γ_1		14818	$91.94\ ^3F_3 + 5.64\ ^3F_2 + 2.19\ ^3H_4$
47	Γ_2		14860	$96.63\ ^3F_3 + 3.17\ ^3F_2 + 0.09\ ^3H_4$
48	Γ_1		14897	$88.59\ ^3F_3 + 9.72\ ^3F_2 + 1.13\ ^3H_4$
49	Γ_2		14914	$97.80\ ^3F_3 + 1.21\ ^3H_4 + 0.59\ ^3H_5$
50	Γ_1	3F_2	15196	$97.65\ ^3F_2 + 1.29\ ^3F_3 + 0.81\ ^3H_4$
51	Γ_1	15116	15342	$87.25\ ^3F_2 + 11.27\ ^3F_3 + 1.28\ ^3H_4$
52	Γ_2		15488	$94.12\ ^3F_2 + 3.30\ ^3F_3 + 2.21\ ^3H_4$
53	Γ_1		15608	$93.97\ ^3F_2 + 3.65\ ^3F_3 + 2.03\ ^3H_4$
54	Γ_2		15638	$98.19\ ^3F_2 + 1.32\ ^3F_3 + 0.29\ ^3H_4$
55	Γ_1	1G_4	21212	$99.78\ ^1G_4 + 0.05\ ^1I_6 + 0.05\ ^1D_2$
56	Γ_2	21374	21263	$99.83\ ^1G_4 + 0.05\ ^3F_3 + 0.04\ ^1I_6$
57	Γ_1		21391	$99.75\ ^1G_4 + 0.08\ ^1D_2 + 0.06\ ^1I_6$
58	Γ_2		21577	$99.87\ ^1G_4 + 0.09\ ^1I_6 + 0.01\ ^3H_4$
59	Γ_2		21614	$99.81\ ^1G_4 + 0.11\ ^1D_2 + 0.03\ ^3F_2$
60	Γ_1		21781	$99.58\ ^1G_4 + 0.17\ ^1I_6 + 0.15\ ^1D_2$
61	Γ_2		21869	$99.64\ ^1G_4 + 0.16\ ^1D_2 + 0.11\ ^1I_6$
62	Γ_1		22041	$99.81\ ^1G_4 + 0.05\ ^1I_6 + 0.04\ ^3H_4$
63	Γ_1		22045	$99.85\ ^1G_4 + 0.05\ ^1I_6 + 0.03\ ^3H_4$

Table 34 (cont'd).
Predicted energy
levels for Tm^{3+} in
 $\text{Ca}_5(\text{PO}_4)_3\text{F}$, C_s site.
 B_{nm} from table 9.

Level	I. R.	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
64	Γ_1	1D_2	28104	$99.78 ^1D_2 + 0.07 ^1G_4 + 0.05 ^1I_6$
65	Γ_1	28032	28135	$99.70 ^1D_2 + 0.13 ^1G_4 + 0.05 ^3F_2$
66	Γ_2		28379	$99.33 ^1D_2 + 0.31 ^3P_1 + 0.21 ^1G_4$
67	Γ_2		28433	$99.54 ^1D_2 + 0.19 ^3P_1 + 0.08 ^1G_4$
68	Γ_1		28557	$99.69 ^1D_2 + 0.13 ^1G_4 + 0.03 ^3P_0$
69	Γ_1	1I_6	34407	$99.75 ^1I_6 + 0.12 ^1G_4 + 0.08 ^3P_2$
70	Γ_2	34886	34408	$99.82 ^1I_6 + 0.12 ^1G_4 + 0.03 ^3P_2$
71	Γ_2	3P_0	34574	$99.87 ^1I_6 + 0.08 ^3P_2 + 0.03 ^1G_4$
72	Γ_1	35637	34587	$99.84 ^1I_6 + 0.10 ^3P_2 + 0.02 ^1G_4$
73	Γ_1		34799	$99.79 ^1I_6 + 0.09 ^3P_2 + 0.07 ^1G_4$
74	Γ_2		34917	$99.66 ^1I_6 + 0.23 ^3P_2 + 0.05 ^1D_2$
75	Γ_2		34981	$99.96 ^1I_6 + 0.02 ^1G_4 + 0.01 ^3P_2$
76	Γ_1		35277	$99.51 ^1I_6 + 0.33 ^3P_0 + 0.11 ^3P_2$
77	Γ_1		35312	$99.85 ^1I_6 + 0.07 ^3P_2 + 0.05 ^1G_4$
78	Γ_2		35852	$99.84 ^1I_6 + 0.10 ^3P_2 + 0.03 ^3P_1$
79	Γ_2		35864	$99.90 ^1I_6 + 0.04 ^3P_2 + 0.03 ^1G_4$
80	Γ_1		35911	$97.65 ^3P_0 + 1.21 ^3P_2 + 0.99 ^1I_6$
81	Γ_1		36146	$99.73 ^1I_6 + 0.14 ^3P_2 + 0.06 ^3P_1$
82	Γ_1		36151	$99.14 ^1I_6 + 0.62 ^3P_0 + 0.13 ^3P_2$
83	Γ_1	3P_1	36315	$99.59 ^3P_1 + 0.18 ^3P_2 + 0.12 ^1I_6$
84	Γ_2	36298	36652	$96.99 ^3P_1 + 2.60 ^3P_2 + 0.30 ^1D_2$
85	Γ_2		36798	$98.72 ^3P_1 + 0.95 ^3P_2 + 0.20 ^1D_2$
86	Γ_1	3P_2	38066	$99.51 ^3P_2 + 0.32 ^1I_6 + 0.08 ^3P_1$
87	Γ_1	38193	38269	$99.51 ^3P_2 + 0.29 ^1I_6 + 0.10 ^3P_1$
88	Γ_2		38520	$97.06 ^3P_2 + 2.61 ^3P_1 + 0.24 ^1I_6$
89	Γ_1		38759	$98.60 ^3P_2 + 1.19 ^3P_0 + 0.10 ^1I_6$
90	Γ_2		38976	$98.74 ^3P_2 + 0.98 ^3P_1 + 0.19 ^1I_6$
91	Γ_1	1S_0	79891	$99.97 ^1S_0 + 0.01 ^3P_2 + 0.01 ^1G_4$
		79592		

^aAqueous centroids (cm^{-1}).

**Table 35. Predicted
energy levels for Yb^{3+}
in $\text{Ca}_5(\text{PO}_4)_3\text{F}$ C_s site.
 B_{nm} from table 9.**

Level	$[(S,L)]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	$^2F_{7/2}$	0	$99.94 ^2F_{7/2} + 0.06 ^2F_{5/2}$
2	250	186	$99.96 ^2F_{7/2} + 0.04 ^2F_{5/2}$
3		702	$99.92 ^2F_{7/2} + 0.08 ^2F_{5/2}$
4		1036	$99.98 ^2F_{7/2} + 0.02 ^2F_{5/2}$
5	$^2F_{5/2}$	10217	$99.96 ^2F_{5/2} + 0.04 ^2F_{7/2}$
6	10450	10694	$99.90 ^2F_{5/2} + 0.10 ^2F_{7/2}$
7		11169	$99.94 ^2F_{5/2} + 0.06 ^2F_{7/2}$

^aAqueous centroids (cm^{-1}).

5. Conclusion

The results of analyzing the optical spectra of Er^{3+} in the two Ca^{2+} sites in $\text{Ca}_5(\text{PO}_4)_3\text{F}$ have been used in the derivation of two sets of crystal-field parameters for the entire series of rare-earth ions, Ln^{3+} . These crystal-field parameters were then used to predict the energy levels of these ions in each of the two different sites: Ca1 (C_3 symmetry) and Ca2 (C_s symmetry). The very large values of the crystal fields (especially the B_{2m} components) cause a very severe mixing of the higher crystal-field energy levels. The mixing is so severe in many of the ions that it precludes completely any purely experimental attempts to analyze the data by analogy to known spectra taken in host materials where the crystal field is much weaker. I hope that the results presented here will serve as a rough guide to experimenters in attempts to unravel their experimental data. In addition to the energy levels, I have used the point-charge model to evaluate the crystal-field components, A_{nm} , and thereby obtained estimates of the Judd-Ofelt intensity parameters, Ω_k . The energy-level eigenfunctions have been used to predict the Zeeman g factors for both sites. These latter quantities may also serve as aids in the interpretation of the experimental data.

References

1. R.W.G. Wyckoff, *Crystal Structures*, **3**, Interscience (1965), 228.
2. J. M. Hughes, M. Cameron, and K. D. Crowley, *Structural Variations in Natural F, OH, and Cl Apatites*, *Am. Mineral.* **74** (1989), 870.
3. D. L. Dexter, *A Theory of Sensitized Luminescence in Solids*, *J. Chem. Phys.* **21** (1953), 836.
4. C. A. Morrison, *Angular Momentum Theory Applied to Interactions in Solids*, *Lecture Notes in Chemistry* **47**, Springer-Verlag (1988).
5. C. A. Morrison and R. P. Leavitt, *Crystal-Field Analysis of Triply Ionized Rare-Earth Ions in Lanthanum Trifluoride*, *J. Chem. Phys.* **71** (1979), 2366. (The $\rho_4(\text{Gd}) = 0.4490 \text{ \AA}^4$, not 0.4990 \AA^4 , as given in table II.)
6. C. A. Morrison and R. P. Leavitt, "Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Materials," in Volume 5, *Handbook of the Physics and Chemistry of Rare Earths*, ed. by K. A. Gschneidner, Jr., and L. Eyring, North-Holland Publishers, New York, NY (1982).
7. T. H. Allik, C. A. Morrison, J. B. Gruber, and M. R. Kokta, *Crystallography, Spectroscopic Analysis, and Lasing Properties of Nd³⁺:Y₃Sc₂Al₃O₁₂*, *Phys. Rev.* **B41** (1990), 21.
8. N. C. Chang, J. B. Gruber, R. P. Leavitt, and C. A. Morrison, *Optical Spectra, Energy Levels, and Crystal-Field Analysis of Tripositive Rare-Earth Ions in Y₂O₃. I. Kramers Ions in C₂ Sites*, *J. Chem. Phys.* **76** (1982), 3877. See also C. A. Morrison, R. P. Leavitt, and D. E. Wortman, *Crystal-Field Analysis of Triply Ionized Lanthanides in CS₂NaLnCl₆*, *J. Chem. Phys.* **73** (1980), 2580.
9. G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups*, MIT Press, Cambridge, MA (1963).
10. J. B. Gruber, M. D. Seltzer, M. E. Hills, T. H. Allik, J. A. Hutchinson, C. A. Morrison, and B.H.T. Chai, *Site-Selective Spectra and Energy Levels of Trivalent Erbium in Calcium Fluorophosphate*, *Opt. Mat.* **3** (1994), 99.
11. R. P. Leavitt and C. A. Morrison, *Crystal-Field Analysis of Triply Ionized Rare-Earth Ions in Lanthanum Trifluoride. II. Intensity Calculations*, *J. Chem. Phys.* **73** (1980), 749.

Appendix A. Selection Rules for Dipole Electronic Transitions in $\text{Ca}_5(\text{PO}_4)_3\text{F}$

Contents

A-1. C_3 Symmetry Site (Ca1)	60
A-1.1 Electric Dipole in C_3 Symmetry	60
A-1.2 Magnetic Dipole in C_3 Symmetry	61
A-2. C_s Symmetry Site (Ca2)	62
A-2.1 Electric Dipole in C_s Symmetry	62
A-2.2 Magnetic Dipole in C_s Symmetry	63

Tables

A-1. Allowed electric dipole transitions for $4f^N$ electronic configuration in C_3 symmetry	60
A-2. Allowed magnetic dipole transitions for $4f^N$ electronic configuration in C_3 symmetry	61
A-3. Allowed electric dipole transitions for $4f^N$ electronic configuration in C_s symmetry	62
A-4. Allowed magnetic dipole transitions for $4f^N$ electronic configuration in C_s symmetry	63

The electric dipole operator, \mathbf{p} , interacting with an external electric field, \mathbf{E} , gives rise to the Hamiltonian

$$H^{ed} = -\mathbf{p} \cdot \mathbf{E} , \quad (\text{A-1})$$

where

$$\mathbf{p} = -e \sum_i \mathbf{r}_i . \quad (\text{A-2})$$

For the magnetic dipole, the interaction with an external magnetic field H is

$$H^{md} = e \left(\frac{\alpha_0}{2} \right) \mathbf{m} \cdot \mathbf{H} , \quad (\text{A-3})$$

where

$$\mathbf{m} = \mathbf{L} + g_e \mathbf{S} , \quad (\text{A-4})$$

and \mathbf{L} is the total orbital angular momentum, \mathbf{S} is the total spin angular momentum, g_e is the free electron g factor, and α_0 is the fine structure constant. For ions occupying either of the sites Ca1 or Ca2 in fluoroapatite, the principal axis is the c -axis of the crystal, which I take as the z -axis in the following. The two types of polarization data, $\mathbf{k} \perp z$ and $\mathbf{k} \parallel z$, with \mathbf{k} the direction of propagation of the fields \mathbf{E} and \mathbf{H} , are referred to simply as the polarization spectra and the axial spectra. The axial spectra arise where $\mathbf{k} \parallel z$ (note that I am considering only propagation along the principal axis so that $\mathbf{k} \cdot \mathbf{E} = \mathbf{k} \cdot \mathbf{H} = 0$). The result with $\mathbf{E} \parallel z$ is referred to as π and with $\mathbf{E} \perp z$ is referred to as σ . (This labeling always refers to the \mathbf{E} vector even for magnetic dipole transitions.)

A-1. C_3 Symmetry Site (Ca1)

A-1.1 Electric Dipole in C_3 Symmetry

The electric dipole interaction can be written

$$H^{ed} = e \left(xE_x + yE_y + zE_z \right), \quad (\text{A-5})$$

where x represents the total x component of $\Sigma_i r_i$ and y and z represent similar abbreviations. From table 42, page 51 of Koster et al¹ (I refer to the tables and pages in this reference in all the following), we have the following:

$$\begin{aligned} x &\rightarrow \Gamma_2 + \Gamma_3, \\ y &\rightarrow \Gamma_2 + \Gamma_3, \\ z &\rightarrow \Gamma_1, \end{aligned} \quad (\text{A-6})$$

and from the group multiplication (Koster et al, table 43), we have the result given in table A-1 for the four types of experimental arrangement. In C_3 symmetry, the Γ_2 and Γ_3 irreducible representations are degenerate, and we label them $\Gamma_{2,3}$. Similarly, for the Γ_4 and Γ_5 , we label them $\Gamma_{4,5}$.

Table A-1. Allowed electric dipole transitions for $4f^N$ electronic configuration in C_3 symmetry.

(a) N even (J integer)

$(\mathbf{k} \perp \mathbf{z})^a$

	Γ_1	$\Gamma_{2,3}$
Γ_1	π	σ
$\Gamma_{2,3}$	σ	π, σ

(b) N odd (J half integer)

$(\mathbf{k} \perp \mathbf{z})^b$

	$\Gamma_{4,5}$	Γ_6
$\Gamma_{4,5}$	π, σ	σ
Γ_6	σ	π

$(\mathbf{k} \parallel \mathbf{z})^a$

	Γ_1	$\Gamma_{2,3}$
Γ_1	0	σ
$\Gamma_{2,3}$	σ	σ

$(\mathbf{k} \parallel \mathbf{z})^b$

	$\Gamma_{4,5}$	Γ_6
$\Gamma_{4,5}$	σ	σ
Γ_6	σ	0

^aApplicable to the following tables in the main body: 14, 16, 18, 20, 22, 23.

^bApplicable to the following tables in the main body: 5, 13, 15, 17, 19, 21, 24.

¹G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups*, MIT Press, Cambridge, MA (1963).

A-1.2 Magnetic Dipole in C_3 Symmetry

The magnetic dipole interaction can be written

$$H^{md} = e \left(\frac{\alpha_0}{2} \right) (m_x H_x + m_y H_y + m_z H_z), \quad (\text{A-7})$$

and again (table 42, page 51 of Koster et al), we have

$$\begin{aligned} m_x &\rightarrow \Gamma_2 + \Gamma_3, \\ m_y &\rightarrow \Gamma_2 + \Gamma_3, \\ m_z &\rightarrow \Gamma_1 \end{aligned} \quad (\text{A-8})$$

(m_i is read as S_i in table 42). Using the multiplication table given in table 43 of Koster et al, we obtain the result given in table A-2.

Table A-2. Allowed magnetic dipole transitions for $4f^N$ electronic configuration in C_3 symmetry.

(a) N even (J integer)
($\mathbf{k} \perp \mathbf{z}$)^a

	Γ_1	$\Gamma_{2,3}$
Γ_1	σ	π
$\Gamma_{2,3}$	π	σ, π

(b) N odd (J half integer)
($\mathbf{k} \perp \mathbf{z}$)^b

	$\Gamma_{4,5}$	Γ_6
$\Gamma_{4,5}$	π, σ	π
Γ_6	π	σ

($\mathbf{k} \parallel \mathbf{z}$)^a

	Γ_1	$\Gamma_{2,3}$
Γ_1	0	σ
$\Gamma_{2,3}$	σ	σ

($\mathbf{k} \parallel \mathbf{z}$)^b

	$\Gamma_{4,5}$	Γ_6
$\Gamma_{4,5}$	σ	σ
Γ_6	σ	0

^aApplicable to the following tables in the main body: 14, 16, 18, 20, 22, 23.

^bApplicable to the following tables in the main body: 5, 13, 15, 17, 19, 21, 24.

A-2. C_s Symmetry Site (Ca2)

A-2.1 Electric Dipole in C_s Symmetry

In C_s symmetry, the components of the electric dipole interaction given in equation (A-5) transform as

$$\begin{aligned} x &\rightarrow \Gamma_1, \\ y &\rightarrow \Gamma_1, \\ z &\rightarrow \Gamma_2, \end{aligned} \quad (\text{A-9})$$

given in table 9, page 33, of Koster et al. Using equation (A-9) and the multiplication table given in table 10 of Koster et al, we obtain the results given in table A-3.

Table A-3. Allowed electric dipole transitions for $4f^N$ electronic configuration in C_s symmetry.

(a) N even (J integer)

$(\mathbf{k} \perp \mathbf{z})^a$

	Γ_1	Γ_2
Γ_1	σ	π
Γ_2	π	σ

$(\mathbf{k} \parallel \mathbf{z})^a$

	Γ_1	Γ_2
Γ_1	σ	0
Γ_2	0	σ

(b) N odd (J half integer)^b

$(\mathbf{k} \perp \mathbf{z})^c$

	Γ_3	Γ_4
Γ_3	σ	π
Γ_4	π	σ

$(\mathbf{k} \parallel \mathbf{z})^c$

	Γ_3	Γ_4
Γ_3	σ	0
Γ_4	0	σ

^aApplicable to the following tables in the main body: 26, 28, 30, 32, 34, 35.

^bIn the double C_s group, the energy levels are all in the degenerate Kramer's doublet $\Gamma_3 + \Gamma_4$, but the tables are useful in the study of the Zeeman effect.

^cApplicable to the following tables in the main body: 6, 25, 27, 29, 31, 33, 36.

A-2.2 Magnetic Dipole in C_s Symmetry

The magnetic dipole interaction given in equation (A-3) has components that transform in C_s symmetry as

$$\begin{aligned} m_x &\rightarrow \Gamma_2, \\ m_y &\rightarrow \Gamma_2, \\ m_z &\rightarrow \Gamma_1, \end{aligned} \quad (\text{A-10})$$

from table 9, page 33, of Koster et al. Using the multiplication table (again the π and σ refer to the *electric vector* being parallel or perpendicular to the z -axis, respectively), we obtain the result given in table A-4.

Table A-4. Allowed magnetic dipole transitions for $4f^N$ electronic configuration in C_s symmetry.

(a) N even (J integer)

$(\mathbf{k} \perp \mathbf{z})^a$

	Γ_1	Γ_2
Γ_1	σ	π
Γ_2	π	σ

(b) N odd (J half integer)^b

$(\mathbf{k} \perp \mathbf{z})^c$

	Γ_3	Γ_4
Γ_3	σ	π
Γ_4	π	σ

$(\mathbf{k} \parallel \mathbf{z})^a$

	Γ_1	Γ_2
Γ_1	0	σ
Γ_2	σ	0

$(\mathbf{k} \parallel \mathbf{z})^c$

	Γ_3	Γ_4
Γ_3	0	σ
Γ_4	σ	0

^aApplicable to the following tables in the main body: 26, 28, 30, 32, 34, 35.

^bIn the double C_s group, the energy levels are all in the degenerate doublet $\Gamma_3 + \Gamma_4$, but the tables are useful in the study of the Zeeman effect.

^cApplicable to the following tables in the main body: 6, 25, 27, 29, 31, 33, 36.

Appendix B. Bibliography of Articles on Fluoroapatites

$\text{Ca}_5(\text{PO}_4)_3\text{F}$, investigated in the main body of this report, is one of the fluoroapatites, a subgroup of the apatites. The fluoroapatites are the most stable and practical apatites for use in lasers and fluorescent light sources. The following bibliography provides a range of references on this useful group.

- Abdulsabirov, R. Yu., and I. N. Kurkin, Parameters of a Crystalline Field at Ca II Positions in Single Crystals of Fluoroapatite, *Opt. Spectrosc.* **32** (1971), 324.
- Aleksandrov, V. I., A. A. Kaminskii, G. V. Maksimova, A. M. Prokhorov, S. E. Sarkisov, A. A. Sobol', and V. M. Tatarintsev, *Stimulated Radiation of Nd³⁺ Ions in Crystals for the ⁴F_{3/2} → ⁴I_{13/2} Transition*, *Sov. Phys. Dokl.* **18** (1974), 495.
- Altchuler, Z. S., S. Berman, and F. Cuttitta, *Rare Earths in Phosphorites—Geochemistry and Potential Recovery*, US Geol. Surv., Prof. Paper 575-b (1967).
- Anderson, J. B., and E. Kostiner, *The Crystal Structure of Cobalt-Substituted Calcium Chlorapatite*, *J. Solid State Chem.* **66** (1987), 343.
- Avanesov, A. G., T. T. Basiev, Yu. K. Voron'ko, B. I. Denker, G. C. Maksimova, V. A. Myzina, V. V. Osiko, and V. S. Fedorov, *Investigation of Spatial Distribution of Impurities in Solids by the Method of Kinetic Luminescent Spectroscopy*, *Sov. Phys. JETP* **57** (1983), 596.
- Bhatnagar, V. M., *The Cell Parameters of Synthetic Calcium Apatites*, *Rev. Roumaine Chim.* **15** (1970), 1735.
- Bhatnagar, V. M., *Preparation and X-Ray Powder Diffraction Patterns of Lead Apatites*, *Chem. Ind. (London)* **48** (1970), 1538.
- Bhatnagar, V. M., *The Cell Parameters of Synthetic Fluoroapatite, Ca₁₀(PO₄)₆F₂*, *Rev. Roumaine Chim.* **15** (1970), 87.
- Bhatnagar, V. M., *The Melting Points of Synthetic Apatites*, *Mineral. Mag.* **37** (1968), 527.
- Daraseliya, D. M., G. V. Maksimov, and A. A. Manenkov, *Relaxation Processes and Discrete Saturation Effects in the EPR Spectrum of Nd³⁺ in Ca₅(PO₄)₃F*, *JETP Lett.* **10** (1969), 229.
- DeLoach, L. D., S. A. Payne, L. K. Smith, W. L. Kway, and W. F. Krupke, *Laser and Spectroscopic Properties of Sr₅(PO₄)₃F:Yb*, *J. Opt. Soc. Am.* **B11** (1994), 269.
- Elliott, J. C., *Recent Progress in the Chemistry, Crystal Chemistry and Structure of the Apatites*, *Calc. Tissue Res.* **3** (1969), 293.
- Engel, G., *Einige Cadmiumapatite sowie die Verbindungen Cd₂XO₄F mit X = P, As und V*, *Zeits. Anorg. Allg. Chem.* **378** (1970), 49.
- Engel, G., *Hydrothermalsynthese von Bleihydroxylapatiten Pb₅(XO₄)OH mit X = P, As, V*, *Naturwiss.* **57** (1970), 355.
- Federov, N. F., I. F. Andreev, A. M. Shevjokov, and T. A. Tunik, *Silicoapatites of Sr and Nb*, *Izvest. Akad. Nauk SSSR, Neorg. Mater.* **6** (1970), 2018.
- Felsche, J., *A New Cerium (III) Orthosilicate with the Apatite Structure*, *Naturwiss.* **56** (1969), 325.
- Fleet, M.E., and Y. Pan, *Site Preference of Nd in Fluoroapatite [Ca₁₀(PO₄)₆F₂]*, *J. Solid State Chem.* **112** (1994), 78.

- Foreman, D. W., Jr., *Neutron and X-Ray Diffraction Study of $\text{Ca}_3\text{Al}_2(\text{O}_4\text{D}_4)_3$, a Garnetoid*, Chem. Phys. **48** (1968), 3037.
- Grisafe, D. A., and F. A. Hummel, *Pentavalent Ion Substitutions in the Apatite Structure. Part A. Crystal Chemistry*, J. Solid State Chem. **2** (1970), 160.
- Johnson, P. D., J. S. Prener, and J. D. Kingsley, *Apatite: Origin of Blue Color*, Science **141** (1963), 1179.
- Johnson, W., *Two Synthetic Compounds Containing Chromium in Different Valency States*, Mineral. Mag. **32** (1960), 408.
- Kaplyanskii, A. A., and E. G. Kuzminov, *Piezospectroscopic Effect and Local-Field Symmetry in Neodymium-Doped Fluorapatite Crystals*, Opt. Spektrosk. **29** (1970), 706 [trans. Opt. Spectrosc. **29** (1970), 376].
- Kaplyanskii, A. A., V. N. Medvedev, and A. P. Skvortsov, *Linear Stark Effect in the Spectra of Fluorapatite Crystals Activated by Rare-Earth Ions*, Opt. Spektrosk. **36** (1974), 368 [trans. Opt. Spectrosc. **36** (1974), 213].
- Klee, W. E., *The Vibrational Spectra of the Phosphate Ions in Fluorapatite*, Zeits. Kristallogr. **131** (1970), 95.
- Klee, W. E., and G. Engel, I. R. *Spectra of the Phosphate Ions in Various Apatites*, J. Inorg. Nucl. Chem. **32** (1970), 1837.
- Klement, R., *Sodium-Calcium-Sulfapatite $\text{Na}_6\text{Ca}_4(\text{SO}_4)_6\text{F}_2$* , Naturwiss. **27** (1939), 568.
- Larsen, E. S., Jr., M. H. Fletcher, and E. A. Cisney, *Strontian Apatite*, Am. Mineral. **37** (1952), 656.
- Lavat, A. E., S. B. Etcheverry, and E. J. Baran, *Crystallographic and Spectroscopic Behavior of Some Mixed Phosphate Vanadate Fluoroapatite*, Z. Naturforsch. **41b** (1986), 987 [in German].
- Levitt, S. R., and R. A. Condrate, Sr., *The Vibrational Spectra of Lead Apatites*, Am. Mineral. **55** (1970), 1562.
- Maksimova, G. V., and A. A. Sobol', *Local Charge Compensation of the Nd^{3+} Ion in Fluorapatite Crystals*, Akad. Nauk SSSR Neorg. Mat. **8** (1972), 1077.
- Maksimova, G. V., and A. A. Sobol', *Nd^{3+} Optical Centers in Crystals of Calcium and Strontium Fluorophosphates*, (1972) Proceedings (Trudy) of the P. N. Lebedev Physics Institute, **60**, pp 59-73.
- Mayer, I., and V. Makogon-Loewy, *Eu(II) -Hydroxyapatite. Preparation and Crystal Data*, Israel J. Chem. **7** (1969), 717.
- Mazelsky, R., R. H. Hopkins, and W. E. Kramer, *Czochralski-Growth of Fluorophosphate*, J. Cryst. Growth **3, 4** (1968), 360.
- McConnell, D., *Infrared Absorption of Carbonate Apatite*, Science **155** (1967), 607.
- McConnell, D., *Crystal Chemical Calculations*, Geochim. Cosmochim. Acta **31** (1967), 1479.

- McConnell, D., *Calculation of the Unit-Cell Volume of a Complex Mineral Structure*, Zeits. Kristallogr. **123** (1966), 58.
- McConnell, D., *Crystal Chemistry of Hydroxyapatite: Its Relation to Bone Mineral*, Arch. Oral. Biol. **10** (1965), 421.
- McConnell, D., *Deficiency of Phosphate Ions in Apatite*, Naturwiss. **52** (1965), 183.
- McConnell, D., and D. W. Foreman, Jr., *The Properties and Structure of $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$: Its Relation to Tin (II) Apatite*, Can. Mineral. **8** (1966), 431.
- Moreno, E. C., T. M. Gregory, and W. E. Brown, *Preparation and Solubility of Hydroxyapatite*, Nat. Bur. Stand. J. Res. **72A** (1968), 773.
- Morozov, A. M., L. G. Morozova, A. K. Trefimov, and P. P. Feofilov, *Spectral and Luminescent Characteristics of Fluoroapatite Single Crystals Activated by Rare Earth Ions*, Opt. Spektrosk. **29** (1970), 1106 [trans. Opt. Spectrosc. **29** (1970), 590].
- Ohlmann, R. C., N. T. Melamed, R. Mazelsky, and W. E. Kramer, *Sensitized Fluorescence of Rare-Earth Ions in Crystals*, Air Force Materials Laboratory, AFML-TR-67-283 (July 1967).
- Prener, J. S., *The Growth and Crystallographic Properties of Calcium Fluor- and Chlor-Apatite Crystals*, J. Electrochem. Soc. **114** (1967), 77.
- Proceedings of the Advanced Solid-State Laser Conference, 7-10 February 1994, Salt Lake City Utah, Opt. Soc. Am., 2010 Mass. Avenue, NW, Washington, DC 20036.
- Shcherbokova, M. Y., L. G. Gilinskaya, and A. A. Godovikov, *Paramagnetic Centers in Apatite*, Kristallografiya **13** (1968), 353 [transl. **13**, 289].
- Simpson, D. R., *Partitioning of Fluoride Between Solution and Apatite*, Am. Mineral. **54** (1969), 1711.
- Simpson, D. R., *Substitutions in Apatite: I. Potassium-Bearing Apatite*, Am. Mineral. **53** (1968), 432.
- Simpson, D. R., *Substitutions in Apatite: II. Low Temperature Fluoride-Hydroxyl Apatite*, Am. Mineral. **53** (1968), 1953.
- St. Náray-Szabo, *The Structure of Apatite $(\text{CaF})\text{Ca}_4(\text{PO}_4)_3$* , Zeits. Kristallogr. **75** (1930), 387.
- Steinbruegge, K. B., T. Henningsen, R. H. Hopkins, R. Mazelsky, N. T. Melamed, E. P. Riedel, and R. C. Ohlmann, *Laser Properties of Nd^{3+} and Ho^{3+} Doped Crystals with the Apatite Structure*, Appl. Opt. **7** (1968), 905.
- Trotter, J., and W. H. Barnes, *The Structure of Vanadinite*, Can. Mineral. **6** (1958), 161.
- Voronko, Yu. K., G. V. Maksimova, and A. A. Sobol', *Anisotropic Luminescence Centers of TR^{3+} Ions in Fluoroapatite Crystals*, Opt. Spectrosc. **70** (1991), 203.
- Wanmaker, W. L., J. W. Ter Brugt, and J. G. Verlijsdonk, *Synthesis of New Compounds with Apatite Structure*, Phillips Res. Repts. **26** (1971), 373.

Appendix B

- Wollentin, R. W., *Lead and Manganese-Activated Cadmium Fluorophosphate Phosphors*, J. Electrochem. Soc. **103** (1956), 17.
- Yefimov, A. F., S. M. Kravchenko, and Z. V. Vasil'eva, *Strontiapatite — a New Mineral*, Dokl. Akad. Nauk **142** (1962), 439 [transl. **142**, 113].
- Yoon, H. S., and R. E. Newnham, *Elastic Properties of Fluorapatite*, Am. Mineral. **54** (1969), 1193.
- Zounami, A., D. Zambon, and J. C. Cousseins, *Optical Properties of Eu^{3+} Activated $\text{Sr}_{10}\text{F}_2(\text{PO}_4)_6$ Elaborated by Coprecipitation*, J. Alloys Comp. **188** (1992), 82.

Distribution

Admnstr
Defns Techl Info Ctr
Attn DTIC-DDA (2 copies)
Cameron Sta Bldg 5
Alexandria VA 22304-6145

Defns Advncd Rsrch Proj Agcy
Attn A Yang
1400 Wilson Blvd
Arlington VA 22290

Director
Defns Nuc Agcy
Attn TITL Tech Lib
6801 Telegraph Rd
Alexandria VA 22310-3398

Ofc of the Dpty Chief of Staf for Rsrch
Dev & Acqstn
Attn DAMA-ARZ-B I R Hershner
Dept of the Army
Washington DC 20310

Under Secy of Defns Rsrch & Engrg
Attn Techl Lib 3C128
Washington DC 20301

Commander
Atmospheric Sci Lab
Attn Techl Lib
White Sands Missile Range NM 88002-5030

Night Vsn & Electro-Optics Lab LABCOM
Attn A Pinto (2 copies)
Attn B Zandi
Attn J Daunt
Attn L Merkel
Attn R Buser
Attn Techl Lib
Attn W Tressel
FT Belvoir VA 22060

Commander
US Army Mis & Munitions Ctr & Schl
Attn AMSMI-TB Redstone Sci Info Ctr
Attn ATSK-CTD-F
Redstone Arsenal AL 35809

US Army Mtrl & Mech Rsrch Ctr
Attn SLCMT-TL Techl Lib
Watertown MA 02172

US Army Rsrch Ofc
Attn G Iafrate
Attn M Strosio
Attn M Ciftan
Attn R Guenther
PO Box 12211
Research Triangle Park NJ 07709-2211

US Army Test & Eval Cmnd
Attn D H Sliney
Attn Techl Lib
Aberdeen Proving Ground MD 21005

US Army Troop Spprt Cmnd
Attn STRNC-RTL Techl Lib
Natick MA 01762

US Frgn Sci & Techlgy Ctr
Attn AIAST-BS Basic Sci Div
Federal Office Building
Charlottesville VA 22901

Nav Rsrch Lab
Attn A Rosenbaum
Attn Code 2620 Tech Lib Br
Attn Code 5554 F Bartoli
Attn Code 5554 L Esterowitz
Attn Code 5554 R E Allen
Attn G Quarles
Attn G Risenblatt
Washington DC 20375

Nav Weapons Ctr
Attn A Wright
Attn Code 3854 M Nader
Attn Code 3854 R L Atkins
Attn DOCE343 Techl Info Dept
China Lake CA 93555

Ames Lab Dow Iowa State Univ
Attn K A Gschneidner Jr (2 copies)
Ames IA 50011

Distribution

Argonne Natl Lab
Attn W T Carnall
9700 South Cass Ave
Argonne IL 60439

Lawrence Radiation Lab
Attn M J Weber
Attn W Krupke
Attn L D DeLoach
Livermore CA 94550

Los Alamos Natl Lab
Attn E T Salesky
505 Openheimer Dr
Los Alamos NM 87544

Oak Ridge Natl Lab
Attn R G Haire
Oak Ridge TN 37839

NASA Langley Rsrch Ctr
Attn C Blair
Attn D Getteny
Attn G Armagen
Attn J Barnes
Attn M Buoncristiani
Attn N P Barnes (2 copies)
Attn P Cross
Hampton VA 23665

Natl Inst of Stand & Techlgy
Attn Lib
Gaithersburg MD 20899

Natl Oceanic & Atmospheric Adm Envir
Rsrch Lab
Attn Lib R-51 Techl Rpt
Boulder CO 80302

Arizona State Univ Dept of Chemistry
Attn L Eyring
Tempe AZ 85281

Colorado State Univ Physics Dept
Attn S Kern
FT Collins CO 80523

Departamento de Química Fundamental &
Departamento de Fisica
Attn A da Gama
Attn G F de Sá
Attn O L Malta
da UFPE Cidade Universitaria
50.000 Recife Pe
Brasil

Howard Univ Dept of Physics
Attn Prof V Kushamaha
25 Bryant Stret NW
Washington DC 20059

Johns Hopkins Univ Dept of Physics
Attn B R Judd
Baltimore MD 21218

Kalamazoo Colg Dept of Physics
Attn K Rajnak
Kalamazoo MI 49007

MA Inst of Techlgy Crystal Physics Lab
Attn H P Jenssen
Cambridge MA 02139

Princeton Univ Dept of Chemistry
Attn C Weaver
Attn D S McClure
Princeton NJ 08544

San Jose State Univ Dept of Physics
Attn J B Gruber
San Jose CA 95192

Seton Hall Univ Chemistry Dept
Attn H Brittain
South Orange NJ 07099

Univ of Central Florida Dept of Physics
Attn B H T Chai
Attn R E Peale
Orlando FL 32816

Univ of Connecticut Dept of Physics
Attn R H Bartram
Storrs CT 06269

Distribution

Univ of Dayton Dept of Physics
Attn S P Sinha
300 College Park
Dayton OH 45469-2350

Univ of Illinois Everitt Lab
Attn J G Eden
1406 W Green Stret
Urbana IL 61801

Univ of Michigan Dept of Physics
Attn S C Rand
Ann Arbor MI 48109

Univ of Minnesota Duluth Dept of Chemistry
Attn L C Thompson
Duluth MN 55812

Univ of South Florida Physics Dept
Attn R Chang
Attn Sengupta
Tampa FL 33620

Univ of Southern California
Attn M Birnbaum
Los Angeles CA 90089

Univ of Virginia Dept of Chemistry
Attn F S Richardson (2 copies)
Charlottesville VA 22901

Univ of Wisconsin Chemistry Dept
Attn J Wright
Madison WI 53706

Université Claude Bernard
Attn R Moncorgé
43 boulevard du 11 Novembre 1918
69622 Villeurbanne
France

UPR 210 CNRS
Attn M Faucher
Attn P Caro
Attn P Porcher
1 Place A Briand 92195 Meudon
France

Allied Signal Inc
Attn R Morris
POB 1021 R
Morristown NJ 07960

Arspec Corp
Attn N C Chang
PO Box 92957
Los Angeles CA 90009

Battelle Pac Northwest Lab Battelle Blvd
Attn N Hess
PO Box 999
Richland WA 99352

Dept of Mech Indus & Arspec Eng
Attn S Temkin
PO Box 909
Piscataway NJ 08854

Engrg Societies Lib
Attn Acqstn Dept
345 East 47th Stret
New York NY 10017

Fibertech Inc
Attn H R Verdin (3 copies)
510-A Herdon Pky
Herdon VA 22070

Hughes Aircraft Comp
Attn D Sumida
Attn MS RL65 R A McFarlane
3011 Malibu Canyon Rd
Malibu CA 90265

IBM Rsrch Div Almaden Rsrch Ctr
Attn R M Macfarlane Mail Stop K32 802(d)
650 Harry Rd
San Jose CA 95120

Inst for Low Temp & Struc Rsrch Polish
Academy of Sci
Attn R Troc
50-950 Wroclaw PO Box 937
ul. Okolna 2
Poland

Distribution

Lawrence Berkeley Lab
Attn N Edelstein
MS 70A-1150
Berkeley CA 94720

LTV
Attn M Kock (WT-50)
PO Box 650003
Dallas GX 75265

Martin Marietta
Attn F Crowne
Attn J Little
Attn P Caldwell
Attn T Worchesky
1450 South Rolling Rd
Baltimore MD 21227

McDonnell Douglass Elect Sys Comp
Attn Dept Y440 Bldg 101 Lev 2Rm/PTB54
D M Andrauskas MS-2066267
PO Box 516
ST Louis MO 63166

MIT Lincoln Lab
Attn B Aull
PO Box 73
Lexington MA 02173

Montana Analytic Services
Attn M Schwan
325 Icepond Rd
Bozeman MT 59715

Sci Applctn Intrntl Corp
Attn T Allik
1710 Goodridge Dr
McLean VA 22102

Southwest Rsrch Inst
Attn M J Sablik
PO Drawer 28510
San Antonio TX 78228-0510

Swartz Electro-Optic Inc
Attn G A Rines
45 Winthrop Stret
Concord MA 01742

Union Carbide Corp
Attn M R Kokta
50 South 32nd Stret
Washougal WA 98671

Univ of Toronto Dept of Physics
Attn D May
Toronto Ontario MSS1A7
Canada

W J Schafer Assoc
Attn J W Collins
321 Ballerica Rd
Chelmsford MA 01824

US Army Rsrch Lab
Attn AMSRL-PS C Thornton
Attn AMSRL-PS M Thompsett
Attn AMSRL-PS T Aucoin
FT Monmouth NJ 07703-5601

US Army Rsrch Lab
Attn AMSRL-PS-AA C Morrison
(10 copies)
Attn AMSRL-PS-AA D Wortman
(10 copies)
Attn AMSRL-PS-AA G Simonis
Attn AMSRL-PS-AA J Bradshaw
Attn AMSRL-PS-AA J Bruno
Attn AMSRL-PS-AA J Pham
Attn AMSRL-PS-AA M Stead
Attn AMSRL-PS-AA M Tobin
Attn AMSRL-PS-AA R Leavitt
Attn AMSRL-PS-AA R Tober
Attn AMSRL-PS-AA T Bahder
Attn AMSRL-OP-SD-TA Mail & Records
Mgmt

Distribution

US Army Rsrch Lab (cont'd)
Attn AMSRL-OP-SD-TL Tech Library
(3 copies)
Attn AMSRL-OP-SD-TP Tech Pub
Attn AMSRL-SS-FA G Turner
Attn AMSRL-SE-RU B Zabudowski
Attn AMSRL-SE-EO C Garvin
Attn AMSRL-SEE-EO J Goff

US Army Rsrch Lab (cont'd)
Attn AMSRL-SSE-RM (A) Chf
Attn AMSRL-SE-RU A A Bencivenga
Attn AMSRL-SE-EP J Nemerich
Attn AMSRL-WT Chf Scentst
Attn AMSRL-WT-NG B McLean
Attn AMSRL-WT-NG Chf